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Determination of Atmospheric Dilution for Emergency Preparedness: A Joint EPA-DOE (Environmental Protection Agency-Department of Energy) Technical Workshop Held on October 15-17, 1986

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A JOINT EPA-DOE TECHNICAL WORKSHOP

OCTOBER 15-17, 1986

Chaired by
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Dr. Harry Moses, U.S. Department of Energy

Edited by
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FOREWORD

This report summarizes the Joint EPA-DOE Technical Workshop Determination of Atmospheric Dilution for Emergency Preparedness, held in Research Triangle Park, NC, at the Meredith Guest House on October 15 and 16, 1986. The individual contributions to this document were prepared from verbatim transcripts of the oral presentations made at the workshop. The transcribed presentations included in this report were reviewed by the authors and their organizations. Several articles were prepared for presentation at the workshop, and these have been included as appendices in this document. In the opinion of the chairpersons, the detail contained in these appendices was important to the overall objectives of the Workshop.

We would like to thank the chairpersons and all who worked to put these proceedings together. Our special thanks go to the editor of this report, Ms. Sharron Rogers at Research and Evaluation Associates, Inc.

Ronald K. Patterson
Project Officer
Atmospheric Sciences Research Laboratory
U.S. Environmental Protection Agency

ABSTRACT

The Joint EPA-DOE Technical Workshop on Determination of Atmospheric Dilution for Emergency Preparedness was held in Research Triangle Park, NC, in October of 1986. The objectives of this workshop were to review the current methods of determining atmospheric dilution for use in hazard identification, emergency preparedness planning, and emergency response, to provide recommendations for choosing among these methods, and, finally, to define the role of the meteorologist in hazard identification, emergency planning, etc. Several invited papers were presented, and panel discussions were held to meet the objectives. The results are presented and discussed.

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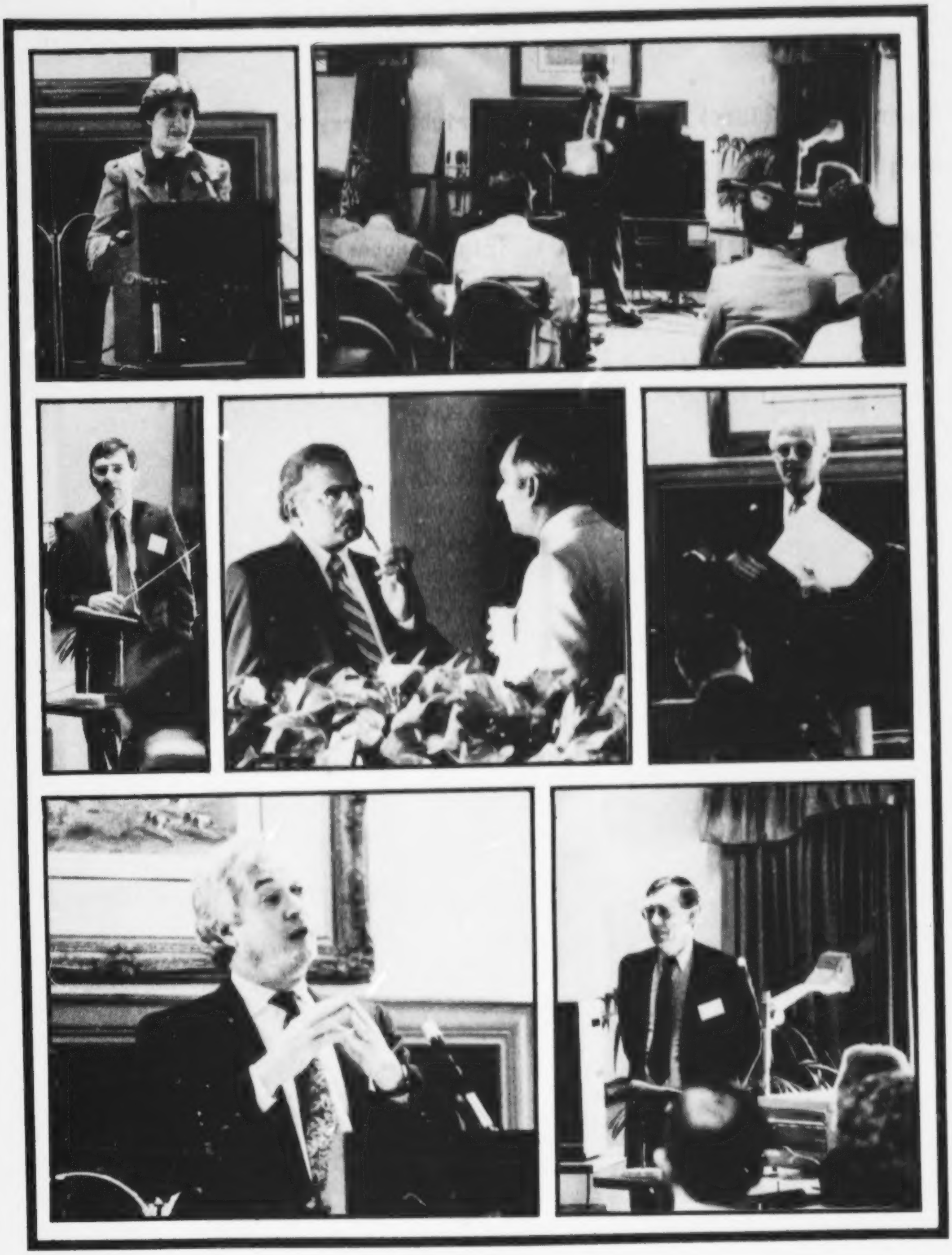

KEY TO PHOTOCOLLAGE OF SPEAKERS

Upper row:	(left) Jane Crum Bare, (right) Jerry Schroy.
Middle row:	(left) Tony Cox, (center) K. Shankar Rao, (right) Marvin Dickerson.
Lower row:	(left) James Makris, (right) Robert Rosensteel.

INTRODUCTION

This workshop was designed as a response to a request from U.S. Environmental Protection Agency (EPA) Headquarters for a forum where the current state of modeling of atmospheric dilution for use in emergency preparedness could be discussed. It quickly became obvious that a joint effort between the EPA and the U.S. Department of Energy (DOE) was the most effective way to proceed. As the designated representatives of the two agencies, we built an agenda for the workshop that would meet the following objectives:

1. To review the current methods of determining the release characteristics, source strength, and rate of dilution of atmospheric contaminants for use in hazard identification and evaluation, emergency preparedness, and emergency response, and to assess the specific strengths and weaknesses for these methods and make recommendations for their improvement.
2. To provide recommendations for choosing among the current modeling methods for immediate use in the identification and evaluation of potential hazards, in the preparation of emergency preparedness scenarios, and in actual emergency response situations.
3. To define the role of the meteorologist in hazard evaluation, emergency preparedness planning, and emergency response.

The participants contributed to these broad objectives from the perspective of their individual situations and experience. One fascinating aspect of the workshop was the interaction between those who had dealt with releases of radioactive material and those who dealt with chemical releases. The radioactive releases have historically involved concerns of large-scale contamination, while the chemical releases have involved concerns of a more local nature. In view of this disparity of scale, it was surprising to see how quickly a common view of the problems associated with potential and actual hazardous releases developed. One strong point of difference was, however, the attitude toward a source term. For radioactive releases, monitoring data taken after the incident will often give a good estimate of the source strength and character. This was shown for the Chernobyl accident.

For hazardous chemical releases, similar monitoring data seldom exist, and sufficient time is seldom available to make such measurements. Only in cases where routine monitoring is done on site is this approach possible for chemical releases. This difference comes from the fact that the hazards of radioactivity were perceived many years ago and appropriate instrumentation developed and installed. It is only recently that the hazards of toxic chemicals have been widely recognized. General agreement has not been reached on the type of on-site measurements necessary, nor in some cases, the need for such measurements.

Because this report consists of transcriptions of oral presentations, no bibliographic citations are given unless provided by the author. To obtain reference information not provided, contact the author.

We wish at this time to express our appreciation to all the participants for their contributions and their patience in the preparation of this document. We wish especially to thank Sharron Rogers, Charlotte Coley, Brenda White, Rebecca Peer, Laura Saeger, Chanya Harris, and Linda Cooper of Research and Evaluation Associates, Inc., who were responsible for the production of the workshop and for

technical writing, editing, and production of this document. We also wish to thank Don Cox of Research and Evaluation Associates, who designed the cover; Mannie Currin, who made the verbatim transcript and had to wrestle with an unfamiliar technical jargon; and the staff of the Meredith Guest House for their help and hospitality.

Francis S. Binkowski
Environmental Protection Agency

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Department of Energy

TECHNICAL OVERVIEW

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In this technical overview for what I consider to be a very important meeting, we need to cover a whole range of topics. What is a source? What is the source of a release of hazardous material into the environment, and how is it characterized? How do the characteristics of sources affect the way that the hazardous material is diluted in the atmosphere? What are the key issues for research today regarding those characteristics and the behavior of hazardous materials? To what use do we put this information when we have that scientific knowledge? What are we really aiming to do in the real world of decision making--both in regulatory decision making and the sort of decision making that industry must do in facility design and siting? Specifically, regarding emergency response planning, we have to address how our knowledge of atmospheric dispersion phenomena can be used in helping us make decisions prior to an emergency and during one.

Examples of Real Sources

First, what is a source? I will be predominantly talking about hazardous chemicals, although others will be addressing radioactive chemicals in this conference as well. The major difference between the two generically is that with hazardous chemicals one typically is concerned only with relatively short-term effects, while radioactive chemicals typically require both short- and long-term concern.

A source that is very typical of hazardous releases into the atmosphere, although an extraordinary one in terms of magnitude, is illustrated by the rupture of a cross-country ammonia pipeline caused by a large bulldozer striking, penetrating, and shearing off the pipeline. An enormous cloud formed. In fact, a cloud of ammonia vapor, ammonia liquid droplets, and condensed water vapor was formed in the atmosphere. This source is not anything like what those of us who work in the field of air pollution dispersion modeling are used to considering. The differences include: 1) it is massive; 2) the cloud emerged under high pressure in a jet-like stream; 3) rapid mixing was induced near the source, particularly at the start of the event; and 4) finally, the cloud becomes denser than air. As the cloud sinks and starts to spread laterally, the emission momentum is lost and the effect of the wind starts to take hold on the behavior of the plume. We must always consider how complicated the phenomena are near a source. They can be very complicated.

A second example is that of a puncture in a chlorine cylinder. This is the small end of the range of events we are considering here. Consider that a very small hole occurs in a 1-ton cylinder, so that the amount of inventory released is not very large. The release occurs as a jet-like plume with a lot of initial mixing. What was the orientation of the release? It could have been horizontal, vertically downwards, or vertically upwards. The hole might have been in the vapor space of the cylinder, or it might have been in the liquid space.

In contrast, the hole in the cylinder could have been large and, thus, the release of the contents of the cylinder could have been essentially instantaneous.

When the brakes failed on a Mexican train comprised of chlorine tank cars, the cars derailed at approximately 80 kilometers per hour and five or six of the cars were ruptured in the resulting pileup. The total amount of chlorine released was about 100 tons. Compared with the previous two cases of holes in vessels, this is an extremely complicated source. One of the tank cars was torn apart, and the release of its contents was instantaneous. While most of the tank cars were caught in the pileup, the head of one car failed and the car rocketed away from the scene, spilling liquid chlorine under pressure behind it. Trying to describe this source of dispersion, we must consider both instantaneous and elongated releases.

When a pipe failed in 1974 in the Flixborough plant in England, a flammable substance, cyclohexane, was released under pressure of about 10 bars. The release occurred as two opposing high-pressure jets with flash vaporizing and aerosol formation; in other words, a very complicated thing from the standpoint of estimating rates of dilution. The result of this particular failure was total destruction of a rather large chemical complex.

Characterization of Sources

Obviously, there are a far wider range of types of releases than these examples cover. A source parameter that is really important to us is the amount of initial dilution that occurs during the quasi-spherical expansion phase of the burst. In the chemical industry, we are dealing typically with materials that are stored under pressure, thus, having a vapor pressure considerably higher than atmospheric pressure. These materials will flash vaporize, and there will be a simultaneous process of flash vaporization and mixing with the atmosphere. The phenomena we can expect to arise are: liquid droplet formation, aerosol formation, liquid droplet coalescence, and rainout of liquid droplets. The liquid droplets, being rather cold relative to the ambient environment, may hit the ground and revaporize or stay there as a liquid pool. These phenomena are extremely complicated and have an important effect on the quantity of material that ends up in the air and, therefore, on the range of hazard faced from such an event.

Transportation container bursts are obviously of a similar character. Another type of rapid, sudden release is the possibility of run-away reactions that can lead to bursting of reactor vessels.

These are all relatively large events. When we look at smaller-scale events, one can list such events as: breakage of pipework, pump seal leakage, discharges from relief valves, and so on. These are also more complex phenomena that result in material being released into the atmosphere without any pressure behind it, such as boil-off from liquid pools or seepage through the ground or through water.

From a real process plant, the releases can take on many forms that seem almost endless. We must describe which of the parameters of these releases are of particular importance to us. Most important is the quantity of the substance that ends up in the atmosphere. When you have a typical chemical release, not all of the chemical ends up in the atmosphere, and there may be many factors that limit the quantity that actually does enter the atmosphere. These factors include orientation of the leak and the presence of any secondary containment.

To consider the effect of orientation, if a liquid were released that is flash vaporizing, but the orientation is vertically downward, it is possible that the flashing two-phase flow will hit the ground, be deflected, and a portion of the liquid centrifuged out. That liquid will cool the ground locally beneath the release point and a pool of liquid will likely form. This situation is even more likely in those cases where secondary containment exists. Conditions such as this are typical of situations where the drain valve of a pressure vessel is somehow stuck open. I submit to you that the processes of liquid fallout from a jet of this sort are not well understood at the present time, and that they are one of the most important subjects of research. People are currently planning and deliberately designing secondary containment in order to have precisely the effect described above.

The quantity of chemical released into the atmosphere also depends on the amount of flashing that is occurring, and how high the vapor pressure of the material in storage is relative to the atmospheric pressure. If it is very high, relatively more of the material will vaporize and more will end up in the atmosphere. Flash vaporization and the process pressure generally both have an influence on what is called initial dilution, either by inducing mixing directly through the turbulence associated with the initial velocity or by the mixing that is associated with the expansion occurring with flash vaporization. Another important modifying factor in actual chemical plants is the presence of obstacles and their effects on initial dilution. An example would be a leak of a fully refrigerated liquefied gas spilled into a bounded area; the presence of an adjacent large tank structure and the effects of the wake of that structure can induce a very large degree of initial dilution of the vapor boiling off from the liquid pool.

All of these factors influencing the amount of chemical released into the atmosphere are extremely complicated. In many cases, the effect of these source-related characteristics on the subsequent dispersion of the cloud is very marked, particularly the effect of the initial pressure. However, this is perhaps more true of flammable than of toxic substances, particularly those toxic materials that are still hazardous at concentrations of the order of only a few parts per million.

Dispersion Modeling

In cases where releases occur with pressure, dispersion models that fail to consider the pressure will seriously overestimate the travel distances of the discharges. In cases where the release occurs without or with almost no pressure, dispersion models, such as typical dense gas dispersion models or even Gaussian dispersion models may be quite relevant to these events.

Please note that the vast majority of hazardous materials are, in fact, in pressurized containment. Therefore, in order for the momentum of such releases to be reduced, one must postulate some continuous mechanism for abstracting the kinetic energy from the initial release. Processes like seepage through the ground or bubbling up through water are the sorts of processes that one has to postulate in order to ignore the effects of the initial momentum when the original source is pressurized.

In the area of subsequent dispersion, those of us who are meteorologists know that the subsequent dispersion is highly dependent on the weather conditions and on factors such as surface roughness and topography. Topography is particularly important because a typical cloud is initially extremely dense relative to the atmosphere and, therefore, particularly strongly affected by topographic effects. In those situations with an absence of topographic effects, such as flat plains, the state of the art in dense vapor cloud dispersion modeling is very well advanced and does not merit very much additional research. Research areas that do require additional attention are the effects of the following: topographic effects on dense vapor clouds, obstacles other than topographic ones, flash vaporization, and rainout.

Hazard Analysis

We need to look for a moment at the uses of hazard analysis and the ways in which the decisions we must make depend on our knowledge of the consequences of hazardous chemical releases. In practice, we find that there are only three uses for hazard analysis for which there is a real need by real decision makers in the real world:

- Land use planning/site selection,
- Plant design, and
- Emergency response.

The first, and most basic, is in zoning and land use planning activities such as selecting a site for a hazardous installation. In such a case, it is obvious that we are dealing with a hazard that has the potential, if the worst were to happen, to have a physical impact over a distance of perhaps several hundred meters. Thus, siting of the facility should be very carefully considered because of the potential risks. The siting decision must involve a balance between the magnitude of the consequences that might occur and the probability of the event occurring. In practice, we find that it is very difficult to site typical industries far enough away from vulnerable populations or other vulnerable entities to eliminate the hazard to the people. In any case, the employees of the facility will be exposed to the risk. Thus, whatever we do about land use planning and site selection, we must accept some residual risk.

There is an analogous argument with respect to plant design (the second of the three uses of hazard analysis). Industries do have an intense interest in designing their facilities to minimize major hazards. They do not want to lose their facilities or injure their employees. They do this not only by site selection, but also by plant layout and by choice of process routes, level of instrumentation detail, emergency shutdown valves, check valves, and other items of this nature, which are really a matter of design detail. Hazard analysis techniques can be, and are being, used to address these detailed matters related to major hazards, but implementing such controls for major hazards may cost money. One can conceive of design features that are impractical simply because they are ludicrously expensive. Those things are not done if it can be shown that the probability of the particular event occurring for which that design provision was being considered was sufficiently low. Thus, there is some acceptance of residual risk.

The third application of hazard analysis techniques, for emergency responses, is the principal topic of our workshop. I would like to make several points about the way I see emergency response fitting into the hazard analysis framework. First, there is one crucial decision that has to be made, how large a physical provision are we going to make for emergency response? How much foam are we going to provide? How much provision needs to be made for breathing apparatus and escape masks? What will be provided to the local population in anticipation of an emergency situation? This type of decision must be essentially risk-based. It definitely is impractical to provide a sufficient emergency response capability to prevent all casualties in the worst possible accident one can postulate. Therefore, we make provisions that fall short of the worst case, and the question is: how far do we go? We make the decision on a risk basis, discounting the worst scenarios provided that we can demonstrate they are sufficiently improbable.

For effective emergency response, we need good preplanning, by evaluation of a representative range of scenarios using dispersion models and tools of that nature. By representative, I mean that we must look at everything from the small leaks to the most extreme cases. Even though we may not be able to cater to the extreme cases, they should be evaluated so that deployment of existing response capability will be the most effective possible. In preplanning for emergency response, the decision-making algorithm is particularly difficult. It is not a simple thing to decide in advance whether the advice given to local populations should be to evacuate or to stay indoors. Depending on the duration of exposure and on the particular chemical released, the advice might be different in different conditions. Such decisions can be very difficult, but can be improved by the prior application of very good models for consequence evaluation.

Whatever emergency plans we select must be extremely practical. The decision-making algorithms have to be presented to the people who will give the orders during the real emergency in such a way that they do not hesitate about the decisions they must make.

Concluding Remarks - Future Priorities

In the recent past, there has been some misdirection of resources by concentrating too much on the niceties of vapor cloud dispersion in the atmosphere. There are in fact many more phenomena that are really involved in chemical hazards than simply the atmospheric dispersion effects. In the future, the balance of effort and interest should be moving towards these other phenomena.

THE BHOPAL GAS TRAGEDY

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In the early hours of December 3, 1984, about 40 tons of highly toxic, volatile, and reactive methyl isocyanate (MIC) gas leaked in about 90 minutes through a 33-meter-high atmospheric vent into the cool night air of Bhopal and quickly spread in a fog-like lethal cloud over a large populated area. Thus began the world's worst industrial disaster, which killed over 2000 people and injured more than 200,000. Here we will sketch the accident scenario and outline the events of the night leading to this catastrophe.

The meteorological and topographical features of Bhopal and the physical, chemical, and toxicological properties of MIC will be described in the context of the cloud dispersion and its effects on human and biological life. A simple analytical dispersion model emphasizing aqueous-phase conversion and deposition of MIC will be presented. This model, based on solution of the atmospheric advection-diffusion equation, gives estimates of ground-level and vertically integrated concentrations. The model estimates qualitatively correlate with recorded human fatalities and injuries and the contours of observed damage effects on trees and vegetation in the affected areas.

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The rehabilitation efforts and some preliminary results of the ongoing medical and toxicological studies will be summarized. We will comment briefly on the legacy of Bhopal, including its implications for siting and operation of plants handling toxic chemicals, worker training, risk assessment and emergency preparedness, occupational health and environmental regulations and enforcement, and other relevant issues.

The city of Bhopal, with a population of about 900,000, is the capital of the State of Madhya Pradesh, India's largest state, with an agriculture-based economy. Bhopal's central location (about 600 kilometers south of New Delhi), communications, resources, and hospitality attracted industry and people from all parts of the country.

Union Carbide, India, Limited (UCIL), which is the corporation involved in this accident, is one of the top 20 Indian companies. They produce about 1500 tons per year of MIC-based pesticides, Sevin (carbaryl) and Temik (aldicarb).

The UCIL pesticide plant is located in the northern part of Bhopal. To the east of the plant is an industrial and warehouse district. To the north are mostly wooded lands that are very sparsely populated. However, the plant is surrounded by residential areas on three sides. Unfortunately, on the night of the accident winds directed the plume toward the populated part of the city.

Bhopal includes hills to a height of about 600 meters and two lakes. It is likely that nocturnal drainage winds and land breezes altered the local surface wind patterns on the night of the accident.

Detailed meteorological data are not available, but various sources indicate that the winds that night were initially from the northwest and subsequently from the north.

There are three MIC storage tanks on the UCIL property. MIC is the raw material used to produce the pesticides carbaryl and aldicarb. At the time of the release, tank 610 contained about 41 metric tons of MIC. A shift change occurred about 10:45 p.m. on the night of December 2, 1984, which was a Sunday. There were about 75 people on duty. The incoming shift was unaware that a runaway chemical reaction was taking place in tank 610.

About 11:00 p.m., the staff noticed the pressure in tank 610 increasing from 3 to 10 pounds per square inch. They mistakenly attributed the increase to nitrogen pressurization of the tank by the previous shift. About 11:30 p.m., the staff noted eye irritation from MIC. Since minor leaks of MIC were not uncommon, they were unconcerned. About 12:00 a.m., they noticed the pressure in tank 610 had increased to 30 pounds per square inch. This was reported to the production supervisor, who checked it almost immediately and found that the tank's rupture disk (designed to rupture at 40 pounds per square inch) had burst, and the safety valve had popped.

At 1:00 a.m., MIC was observed to be escaping through a 33-meter high atmospheric vent line into Bhopal's cool night air. Within a 90-minute period, about 40 tons of gaseous MIC leaked out. None of several plant safety systems in place fully functioned that night. A scrubber, charged with caustic soda, contained only enough to neutralize about 7 tons of MIC released. A flare tower did not work because it was undergoing maintenance. A water curtain designed to hydrolyze escaping MIC reached only a height of 15 meters, far below the release point. The facility's refrigeration plant was down.

The public siren was turned on for a few minutes at 1:00 a.m., but was not sounded again until 2:00 a.m., to alert the public to the danger. By then, thousands of people were fleeing.

About 200 people died in their beds in the immediate vicinity of the plant where a huge white cloud formed and moved southward towards the densely populated areas. Near the plant, the gas was so thick that visibility was very low. These people awoke to a nightmare of suffocation, burning eyes, and panic. They rushed out into the streets to join thousands of other people who were running for their lives. Many people became overcome by fumes and collapsed along the way. Rescuers converged on the area around 1:30 a.m. By dusk of that first day, the death toll mounted to about 1000 and over 100,000 were injured. As the magnitude of the disaster became apparent, medical equipment and relief were rushed to the stricken city.

MIC is known to be a very reactive, toxic, and volatile chemical. It undergoes exothermic and vigorous reactions with a variety of compounds containing active hydrogen atoms. Analysis of sludge from tank 610 after the accident showed that two major exothermic reactions took place. One was MIC reacting with water; the products of MIC hydrolysis with water made up 16 to 28 percent of the samples. The second, and much faster reaction, was MIC reacting with itself, catalyzed by iron. More than 50 percent of the sludge consisted of MIC trimer resulting from this second reaction. A small amount of water with a trace of contaminants, such as rust or salt, could catalyze an autoreaction. The heat liberated during an induction period lasting a few hours could generate a reaction of explosive violence. It is not inconceivable that a small trace contamination could have occurred in the MIC tank in spite of the best prevention efforts.

Once gaseous MIC escaped into the air, it would undergo advection, diffusion, and chemical transformation, with atmospheric moisture. The major reaction product would be methylamine, which is absorbed and stays in the soil until slowly broken down by biological reactions and weathering.

We used an analytical dispersion model based on the atmospheric advection-diffusion equation. The source strength was established at 40 metric tons in about 90 minutes. MIC vapor is twice as heavy as air. This suggests that density effects might be important for plume dispersion. However, the vapor escaped at a very high velocity, which leads to considerable entrainment. Also, the reaction of MIC with moisture releases about 1.36 x 10^6 joules per kilogram of heat that reduces the plume density. With these considerations, the density effects were not considered, but gravitational spreading was included. Post-episodic reconstruction of the accident by scientists established that the wind was initially northwesterly during the accident, and subsequently northerly.

According to our model, most of the high concentrations occurred in the first kilometer southeast of the plant. A region extending about 7 kilometers downwind of the plant was affected. Birds, cattle, cats, dogs, goats, and all other animals were killed over a 65-square-kilometer area in the southeast quadrant of the plant. Based on the model estimates, we have divided the affected area into four zones. Zone 1 consists of concentrations >50 parts per million, zone 2 consists of concentrations >15 parts per million, zone 3, >1.5 parts per million, and zone 4, <1 part per million. In the first few hours after the accident, zone 1 (severely affected) out of a population of 6173, sustained 360 fatalities. Initial fatalities in zone 2 (with a much larger population) amounted to 508. In zone 3, there were about 11 initial fatalities, and in zone 4, about 5. The correlation with the fatalities provides some indirect evidence that these concentration estimates are reasonable, although the large population movement that night makes these comparisons somewhat subjective. Most of the fatalities, however, occurred close to their place of residence.

Perhaps the best concentration monitors for the effects of the accident at Bhopal are the plants and vegetation in the area. The Indian Agricultural Research Institute and the Central Board for Control of Pollution conducted a vegetation damage survey that showed most of the effects occurred in the southeast, southern, and eastern directions from UCIL's boundaries. The same species were affected differently depending on location relative to the plant and the amount of moisture available in the ground at the time of exposure. Vegetation that had been irrigated on the previous day was much less affected. Some tall trees were completely defoliated. Much of the vegetation in affected areas looked as though it had been burned. Additional detailed studies are still under way to study the impacts on the vegetation. Studies are addressing the histological effects on the lipids of the leaves and on the microorganisms attached to the foliage.

Very little is known about MIC's toxicological effects, especially the long-term ones. What little data are available were from tests done on rats. The permissible MIC skin exposure limit, a voluntary standard, is 0.02 parts per million. This is the amount of MIC to which a person can be safely exposed over an 8-hour workday. This threshold limit value (TLV) has been set by the American Conference of Governmental Industrial Hygienists (ACGIH). The lethal dose is estimated to be between 15 and 30 parts per million, depending on age and sex. Before the Bhopal episode, the effects of MIC had never been observed on such a large and diverse population. Isocyanates were known to attack the respiratory system, eyes, and skin.

Laboratory analyses have confirmed that most of the deaths in the immediate vicinity of the plant occurred from cyanide poisoning. Cyanide was probably released because of the high temperatures reached in the MIC tank, causing the MIC to break up into hydrogen cyanide, methylamine, carbon monoxide, and other organic cyanide products.

While it will be some time before the studies at Bhopal are completed, clinical and toxicological studies are being coordinated by the Indian Council of Medical Research. Medical treatment has dramatically improved the condition of people with eye injuries. Lung problems persist in many victims. A large number of victims with pulmonary edema have recovered, but many were left with considerable damage to their small airways and alveoli. Children were the worst affected, with about 39 percent showing moderate to severe pulmonary disability. Miscarriages and stillbirth were frequent in the pregnant women exposed to the gases. In the first 20 weeks, 436 spontaneous abortions occurred out of 2600 pregnancies; the normal rate for Bhopal was 6 to 10 percent.

On the night of the accident, the doctors of Bhopal, supported by medical students, interns, and the nursing staffs, rallied to respond to this unprecedented, sudden disaster. Because there was so little known about the toxicology of MIC and its reaction products, the medical personnel had to improvise in the beginning. There certainly was and is a real need for information on the processes, potential hazards, biological effects, and the medical treatments that should be made available in any kind of industry involving toxic chemicals.

The Union Carbide plant was located close to the population in Bhopal. There should be at least a 2- to 3-kilometer buffer zone between hazardous industries and the population centers. Standards, enforcement, safety, health, and environment are very important.

Bhopal offers many lessons that have to do with basic human concerns for safety. If these lessons are lost, it is all too likely that an accident like this can happen again.

Note: A prepared paper by the authors on this topic appears in Appendix A.

NATIONAL RESEARCH NEEDS FOR EMERGENCY RESPONSE IN THE WAKE OF CHERNOBYL

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The material presented today is a distillation of materials from about 3 feet of shelf space. We will consider what actually happened at Chernobyl, the nature of the warning that the free world received, and how that warning came. The first tasks that then faced the United States were assessment and making sense out of the inconsistent and sometimes conflicting information.

First, let us briefly review the setting of the Chernobyl accident. The reactor, in operation approximately 2 years, was a 1000-megawatts (electric) generating plant with about 3200 megawatts of thermal energy. The reactor is graphite moderated, water cooled, and has confinement, but not containment in the United States sense of this term. The reactor core is in an interior building with what the Russians call a protective shield around it, built of steel and surrounded by an inert gas. Thus, there is or was a barrier between the oxygen in the confinement building and the material inside the reactor.

The accident sequence has been covered in detail in various publications and will not be repeated here. During the turbine experiments and the shutting down of the safety devices, there was an excursion and a gradually increasing instability of the reactor with a large steam pressure buildup inside the interior structure. In the interior of the reactor, inside of the protective shield, a pressure of over 1000 pounds per square inch ripped off the tops of some 1650 pressure tubes exposing the graphite and fuel elements to the atmosphere. Shortly thereafter, the graphite, which was at 750°C, ignited. As a result of the preceding explosions, the plumbing and instrumentation were probably disrupted. At that time, water and steam could readily contact the zirconium, and water and steam could also contact the hot graphite, generating large amounts of hydrogen and carbon monoxide, both combustible. The source term at Chernobyl can be described as a chaotic fire, multiple explosions, gas generation, and various sources of water contacting the hot graphite. In terms of initial distribution of the released inventory, we must think of burning gases, burning graphite, burning carbon monoxide, and perhaps multiple explosions, driving a plume up through the atmospheric boundary layer. This is an "image" of Chernobyl at 1:23 a.m. on [Saturday,] April 26, 1986.

Our first warning came from Scandinavia late Sunday and on Monday morning. We learned by telephone that a suite of radionuclides were being observed on particulate filters in Scandinavia; radioiodines and radiocesiums were present in copious amounts. Other isotopes (e.g., ^{60}Co) were coming from neutron activation of the cooling system, which confirmed a disruption and at least partial destruction of this system. The particles of ruthenium were spherical, suggesting that at least part of the fuel released had seen temperatures of 2500°C. (Later interpretations indicate that the Ru particles came from shattered fuel elements entrained into the plume or explosively injected into the atmosphere.) From the ratios of ^{137}Cs and ^{134}Cs, a reactor source term could be identified, and the time of shutdown of the plant deduced. Obviously, all of these deductions were not completed on Monday, but they were possible to obtain later from those first samples.

Lawrence Livermore National Laboratory (LLNL) used modern particle-in-cell techniques in three dimensions over spatial scales of thousands of kilometers to deduce the long-range transport and dilution. We also used (as an independent check) Lagrangian large cloud simulation models for transport and dispersion. These later models are 15 to 20 years old and were developed for the atmospheric nuclear test events. These models have been used many times, and we know their degree of confidence and their performance levels. The diagnostic models were zoned to make sense out of the available information. Nested grids were used for the area of Europe and the Soviet Block countries. The remote grid zones were 48 by 48 kilometers on the horizontal plane, and nested down to approximately 3 kilometers on the side in areas surrounding the Chernobyl plant. To do the simulations, this grid pattern was used for the diagnostic flow fields in three dimensions fitted to the observations over Europe. Particle-in-cell calculations were driven by those flow fields to determine subsequent dilution, not initial dilution, of the released materials.

The first model calculations allowed the development of an estimate of the dilution factor, X/Q, at the points of observation/measurements in Sweden and Finland. By dividing the observed concentrations by the dilution (X/Q), the source term and rate of release could be estimated. This was done for a number of stations along the route of cloud passage, and an estimate of the curies by isotope that were released into the atmosphere was developed. Nuclear engineers from both the civil and military communities made estimates of the core inventories and the relevant nuclides of greatest interest. At the time of reactor shutdown, 80 million curies of ^{131}I were estimated in the core inventory with 6 million curies of ^{137}Cs. During the first 24 hours, it is estimated that all of the noble gases were released when the 1650 pressure tubes were destroyed. A high fraction of the volatiles were released. Our assumption is that 40 percent of the volatiles were released on the first day into the Zone A cloud and 10 percent into that zone on each of the subsequent 5 days. The amount of material going into Zones A and B of the cloud over the 6-day period was developed from experience based on fallout clouds. However, these estimates were checked by cumulus cloud simulative models that normally use a radius of 5 kilometers for the scale of the base of the cloud. The Chernobyl fire plume was approximately 20 meters in radius--the world's smallest convective column; it was driven by a flux of 62 megawatts across the surface of the 20-meter radius.

Over 100 maps of material dispersed and deposited over Europe and Asia were generated in the simulations. One of these maps shows the integrated exposures to an individual standing in the path of the plume at 2 days (48 hours) after the accident. The highest calculated dose was 133 rem to the adult thyroid in the vicinity of the plant. The exposures at the distance of the coast of Sweden were equivalent to 0.1 rem at the end of 48 hours. From these simulations, it was learned how Kiev was fortunate, indeed. The plume from the accident rose up over a relatively dry warm front, so there was not much of a problem from rainout of radioiodine. There was, however, significant convective activity in the area of Kiev at the time, although the plume was not significantly impacted by that activity. Observations in Sweden were significantly affected by the lifting of the plume over the warm frontal area in the region of the Baltic Sea.

The results of the LLNL simulations were sent to the President's Commission through the Department of Energy. These results are in relatively good agreement with the calculations and observations of Scandinavia and Eastern and Southern Europe, that is, by a factor of two with measured values for deposition by isotope. Agreement was not good in Western Europe, possibly due to the gliding up over the warm front (later calculations show better agreement when meteorological data from all of Western Europe were used). The calculations and measurements showed that there were no acute health effects outside of the Soviet Union.

To put Chernobyl in perspective, the accident was compared to a 20-kiloton nuclear test and the released inventory of the Three-Mile Island (TMI) reactor accident in the following table. The estimated

COMPARISON* OF CHERNOBYL WITH OTHER RADIONUCLIDE RELEASES

Nuclide	Chernobyl	TMI	20-kiloton Nuclear Test
^{131}I	10-50	.00002	2
^{137}Cs	1-6	None detected	.004
^{90}Sr	.001-.07	None detected	.004
Noble gases	100-200	10	5

*Megacuries of radioactivity 3 days after shutdown or test.

release inventories for Chernobyl indicate that radioiodine releases were approximately 20 times greater than at a 20-kiloton nuclear test. No cesium was detected at TMI; it stayed inside the containment. No ^{90}Sr was detected at TMI, but was at Chernobyl. While virtually all of the noble gases were released at TMI and Chernobyl, the amount was far smaller at TMI. The differences in long-term dose occur because the dose at TMI came mainly from the noble gases, while the long-term dose at Chernobyl comes mainly from the ^{137}Cs. The maximum individual dose at TMI was 11.5 millirems, while the maximum dose at Chernobyl was above the lethal dose for half the exposed population (LD_{50}), delivered by fission products, not the noble gases. Rainout was not important at TMI because noble gases are not scavenged. At Chernobyl, the iodines were scavenged and are of continued importance to the Soviets. The hot spots in Europe were created by rainout. These rainout hot spots run roughly 10 times above areas subject to dry deposition alone. The message from these findings is that containment, design, and safety devices are immensely important in terms of explaining the differences between Chernobyl and TMI. All of the diagnostic work shown today in this presentation was completed in the first 14 days following the event and reported to the President's Commission.

The New York Times reported that Chernobyl released much more radioactivity than all of the atmospheric testing by both of the super powers. It is important that we understand that this was an error. The correct number is that Chernobyl's release of ^{137}Cs is 6 percent of the ^{137}Cs released from super power testing.

In preparing to model the upper cloud from Chernobyl, we quickly learned that we did not need the whole radioiodine inventory to explain the readings in Scandinavia. So the question was, where was the other half of the radioiodine? It would have been easy to say that the models were no good, but this was not the reason. When the United States' sophisticated sampling aircraft measured radioiodine at 5500 meters above Japan, we quickly redirected our focus. Taking the long-range transport models from nuclear test days and back calculating from Japan, we found that half the radioiodine had to be at higher elevations over Chernobyl on the first day. Calculating forward from Japan, it was possible to estimate how much radioiodine would be measured off the coast of California when the cloud began its passage over the United States. The models estimated that 30 picocuries per cubic meter would be found at the California coast. On cloud arrival, the aircraft measured 12 picocuries per cubic meter. That is a reasonable comparison in this business. We now believe that an upper cloud was created by the early explosions, the intense fire, and residual heat from the reactor. A lower cloud was produced by the lingering fire that had a lower heat flux.

From the California coastal estimate, transport was projected over the continental United States, assuming a reasonable vertical distribution, calculating a vertical integral, and assuming immediate scavenging of 100 percent of the vertically integrated iodine. Assuming this radioiodine to be deposited on the ground and eaten by the family cow, the maximum amount of radioiodine in cow's milk in the United States was estimated to be approximately 900 picocuries per liter. As you will recall, guidelines are established at 15,000 picocuries per liter. Thus, we estimated that there would be no health problems in the United States as a result of radioiodine deposition, even in the deposition hot spots. In areas actually measuring radioiodine concentrations in milk, the maximum measured was 600 picocuries per liter in one sample. Most of the measurements were from 100 to 200 picocuries per liter or less across the United States. From these simulations and the many measurements, we believe that the upper cloud from Chernobyl did exist.

From all of the northern hemispheric measurements and simulations, we now estimate that there were 2.4 million curies of ^{137}Cs released, which represents just less than half of the core inventory. Approximately half of the ^{131}I inventory of 80 million curies, or 47 million curies, was released. Our final estimate is that half of the core inventory of cesium and iodine was released with 100 percent of the noble gases, 10 percent or less of the tellurium, and 1 percent or less of the other materials.

The experiences from Chernobyl lead us to identify several research needs. One of the most important things we can do to improve emergency response is to improve the flow of information. This means early warning by the country involved with the accident; openness concerning what was released, the nature of the accident, severity and early measurements; in fact, everything known about initial distribution of the material released. In the United States, we need to improve our own flow of information. There are nine Federal agencies involved in emergency response. Each one claims a role, does quality control differently, and perceives a different jurisdiction.

Additional research is also needed in the area of meteorological prediction. Models can be driven with input from numerical weather prediction models that operate on the global scale down to mesoscale models on the smaller scale, i.e., state-size, regional-size, or continental in scale. Yet, each serves different purposes. On the larger scale, for a massive event like Chernobyl, the question is where is the released material going and what will the concentration be when it gets there? For smaller chemical releases, the prediction serves a different purpose. You may have a hazardous condition to engineer your way out of and, through prediction, one can select optimal conditions in which the material may not flash, or other risks can be minimized. Thus, prediction serves different purposes depending on the manager's and decision maker's needs.

We need to know the physics and chemistry of the release. At Chernobyl, we needed to know the combustion products, the heat fluxes, and the isotopes released to the environment, in order to know what the exposure and doses to man would be. To say so many curies of activity are released is meaningless. You must know the number of isotopes and the amount of each isotope in order to know the mode of exposure and those doses that will finally be delivered to the human community.

Our particle-in-cell techniques need to be expanded to handle complicated and differing sets of isotopes. It is easy to do particle-in-cell calculation for one to five different isotopes. To do simulations for a suite of 15, 16, 40, or 50 and do these calculations quickly, requires improved techniques. We would call this improvement a hybrid particle approach. In the last 5 years, two proposals have been developed to address this specific need, but have not been funded (by any Federal agency).

We need additional information about scavenging properties. The radioiodine from Chernobyl was carried on a host aerosol. Iodine exists both in gaseous and particulate form as it moves downwind. The scavenging is mainly of the particulate. It can be scavenged very efficiently if the iodine is coating the host aerosol particle, because iodine is a cloud-seeding material and is most effective in the ice-producing parts of clouds, which probably existed over Europe and Japan where the "hot spots" were created by wet deposition.

We need standardization of action levels of contamination in products to know what actions to take consistently. In Europe, part of the confusion was due to the lack of uniformity of standards. Vegetables were needlessly destroyed, and populations were needlessly disturbed. The countries tended to overreact because of nonuniformity of standards and extremely low standards set by people who wanted to show what good they were doing for the environment. When, in fact, it became "crisis time," they created confusion in the population. The Soviets claimed that no damage occurred outside their country and that the Westerners took unnecessary precautions. Yet, some Westerners, such as the shepherds of Wales, are seeking compensation from the Soviet Union. Such compensation will not be possible in international law circles until there is standardization of action levels and protective action guides. There needs to be standardization of measurements, analysis, and reporting procedures. A specific problem with reporting occurs with iodine levels. When a given iodine level is reported from a specific station, one must also know how it was measured. It makes a difference whether the iodine is a gas or attached to particulates.

We need to study the biomedical history of the 200,000 severely dosed people in the Soviet Union. This is not the acute radiation victims who saw more than a few hundred rem in the first day or so after the Chernobyl accident; they will certainly be studied. The 200,000 who saw from 50 down to a few rem should be medically tracked and will constitute a valuable database for understanding radiation effects.

The Soviets proved to be ingenious in minimizing the impacts of the accident. We should learn from how they did it. They minimized resuspension of the radioactive material in the deposition pattern around and up to some distance from the plant. They controlled runoff to the streams and reservoirs by building levies so as not to contaminate the water resources of the city of Kiev. They did rainfall suppression in the region of Kiev in order to reduce the problem of surface runoff in the neighborhood of the plant. They also took other actions too numerous to list here.

There is one area where the Russians were very lucky. The initial plume from Chernobyl went northwest to an area of relatively uninhabited boreal forest. As a result, a relatively large fraction of the release inventory is resting in and on the pine needles of the boreal forest some meters above the ground. As the pine needles die from the beta radiation, they will fall as fallout during the next several years northwest of Kiev. This is an ideal laboratory for the study of long-term ecological effects of radiation, which the world has not seen.

Thank you very much. This discussion outlines my ideas of research needs in the wake of Chernobyl.

ACCIDENTAL RELEASE SCENARIOS FOR ANALYSIS

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Accidental releases are a new area of study with most activity occurring in the United States only since the 1984 accident at Bhopal, India, where approximately 2500 people were killed and thousands more injured. Until this accident, very little recent effort was put into modeling the dispersion of acutely toxic gas clouds that could cause effects due to short-term emissions. The purpose of this workshop is to gather expert dispersion modelers to analyze various scenarios. The purpose of this paper is to provoke this discussion and present actual scenarios for analysis. The specific subjects discussed were chosen by those organizing the workshop who felt that the attending dispersion modelers needed a background in this area to which they might not have had previous exposure. The first section will discuss past releases that have occurred in the United States. The second section will provide more of a statistical side by presenting chemicals most frequently involved. The third area will discuss some of the many variables that affect source strength and dispersion modeling, and the final section will present three representative scenarios for analysis at the workshop. None of these sections will provide an exhaustive account of the topics, but will simply touch on major points.

Case Histories

Several questions were presented for this section. These questions included: Have acutely toxic chemicals similar in toxicity to methyl isocyanate (MIC) been released in quantities comparable to the quantities released in Bhopal? Has anything equivalent to Bhopal happened in the United States in the past? Are releases occurring today? To find the answers to these questions case histories were reviewed.

Have acutely toxic chemicals similar in toxicity to MIC been released in quantities comparable to the quantities released in Bhopal? EPA's Acute Hazardous Events Database contains a computerized record of 6928 incidents that have occurred in the United States in the last 6 years. The toxic load was calculated for Bhopal and 300 other events in the database, where toxic load is defined to be the amount of chemical released divided by the IDLH (immediately dangerous to life and health) of the chemical. For Bhopal, approximately 90,000 pounds of MIC was released, where MIC has an IDLH value of 43 milligrams per cubic meter. This corresponds to a toxic load of approximately 2100 pounds of MIC per IDLH value. IDLH represents the maximum level at which a healthy male worker could escape after 30 minutes exposure without irreversible effects or loss of life. Some chemicals without established IDLH values use calculated IDLH from other health effects data. Here the IDLH is expressed in units of milligrams per cubic meter for consistency in the toxic load calculations.

Six events within the database were determined to have toxic loads greater than Bhopal's. In other words, if all other factors had been equal (e.g., population density, meteorology, physical state, and emergency response), these events would have represented at least as much potential for toxic effects as the event at Bhopal. In each of the six cases, however, the factors were not equal and not a single life was lost.(1,2)

Has anything equivalent to Bhopal happened in the United States in the past? In doing research, the following three events seemed not of equal magnitude, but had serious consequences.

- Cleveland, OH, October 20, 1944. A liquid natural gas storage tank ruptured at 5 pounds per square inch and -250°F in a residential and industrial area. Liquid natural gas flowed down the storm sewers, mixed with air, and exploded. A total of 128 people were killed, and 200 to 400 were injured.
- Texas City, TX, 1947. Bagged ammonium nitrate fertilizer on board a ship caught fire; 2280 tons of fertilizer burned and a nearby ship exploded. After the explosion and fires, 330 dwellings, 130 business buildings, and 600 automobiles had been destroyed. A total of 3000 people were injured, and 552 lost their lives.
- Brooklyn, NY, 1944. Chlorine was released from a gas cylinder into the subway system. A total of 208 people were injured; no one was killed.(3)

These events happened approximately 40 years ago. Are releases occurring today? The following events from the Acute Hazardous Events Database occurred within the last 6 years in the United States.

- Niagara Falls, NY. One ton of liquid chlorine spilled from a process vessel in a chemical plant. The plume that followed resulted in the evacuation of a nearby sports stadium where a game was in progress. A total of 76 people were injured.
- Elizabeth, NJ. At the Newark Airport, a release of isobutane, phosgene, hydrogen chloride, and hydrogen cyanide

resulted in the evacuation of the entire airport and 15 miles of the New Jersey Turnpike.

- San Francisco, CA. A liquid and gaseous release of polychlorinated biphenyls (PCBs), natural gas, and oil resulted in the evacuation of 19 buildings containing 30,000 people at the time.(1)

Event Statistics

What are the statistics? What are the chemicals most frequently involved in releases?

The best source of information at this point in time for data on accidental releases in the United States is the Acute Hazardous Events Database. The database provides an analysis of the frequency with which chemicals are involved in fatal and injurious events, the causes of the events recorded in the database, and the locations of the releases. Even this database has many caveats associated with it, however. For example, the deaths and injuries may not be related directly to exposure to toxic substances, but may have resulted from collision, fire, explosion, or other related causes. Also, the method of collecting the data may have been biased more toward significant events, rather than toward less significant events. This database may not have statistical significance, but this is the best source of information available at this time.

What do the data indicate? For events causing death or injury, chlorine was the chemical released in 9.6 percent of the cases, anhydrous ammonia was released in 6.8 percent, followed in decreasing frequency by sulfuric acid, PCBs, hydrochloric acid, nitric acid, toluene, methyl alcohol, and sodium hydroxide.(1)

Range of Release Characteristics

What are the ranges of parameters that need to be considered when modeling an accidental release? Some of the major factors in chemical releases are: the chemicals involved, the physical state of the chemicals, the conditions of release, and meteorological data. Most source strength and dispersion modelers are familiar with the differences due to different chemicals and meteorological data, but may not be familiar with some of the physical states and conditions of accidental releases.

The physical state includes solids, liquids, gases, or two-phase releases. Low boiling point liquids are known for a slow, steady evaporation rate. Superheated liquids and refrigerated gases are known to have an initial flashing condition, and then a steady rate of evaporation. After evaporation takes place, liquid spills may be modeled as light, neutrally buoyant or dense gases, depending on the characteristics of the gases formed. Usually, the heavier-than-air clouds are considered the most serious because they tend to stay near the ground and, thus, in the breathing zone of the surrounding populations. Sometimes, however, due to meteorological conditions, lighter-than-air gases can act as heavier-than-air gases and then warm up to be neutrally buoyant and then lighter-than-air gases.

Two-phase releases are mixtures of gases and liquids. These often result from a safety valve release from a high-pressure vessel or an explosion in a chemical plant. A boiling liquid expanding vapor explosion (BLEVE) is a subset of this group. Solids can be divided into four major groups: powders, molten solids, solids in solution, or brick-like solids. Of these, powders often pose the largest problem in terms of fires and explosions, while brick-like solids are very rarely considered a problem.

Many other parameters affect short-term releases, including: unexpected reactions (including products of combustion, which may themselves be toxic) and characteristics of the release (e.g., jet vs. passive releases). For more information on factors involved in accidental releases or equations used to describe releases, see the book by Frank Lees, Loss Prevention in Process Industries.(3)

Representative Credible Scenarios

The final purpose of this paper was to establish credible scenarios for analysis at the workshop. The scenarios chosen are all historical accounts from a review of individual articles, the Acute Hazardous Events Database and the Loss Prevention in Process Industries by Frank Lees. These cases represent some of the worst situations involving the chemicals chosen.

The first scenario is a chlorine release. Chlorine is a heavier-than-air chemical involved in 9.6 percent of the accidents in the Acute Hazardous Events Database and has been credited with causing

2 deaths and 382 injuries.(1) Chlorine is stored as a liquefied gas in amounts up to 450 tons and in larger quantities at low temperatures and atmospheric pressures.(4) On December 10, 1976, chlorine was released in Baton Rouge, LA, at a plant undergoing start-up after shutdown for maintenance. An explosion overturned the tank, puncturing its sidewall on a sharp object. Over the next 6 hours, 100 tons of chlorine were released.(3) What model would be recommended for the emergency response personnel making evacuation/shelter-in-place recommendations?

The second case study involves an ammonia release. Ammonia was the third highest chemical in production in 1985.(5) It is credited with 271 injuries and 4 deaths in the Acute Hazardous Events Database.(1) Ammonia is lighter than air but can act as a heavy gas in very cold conditions.(3) The Mid-America Pipeline system crosses seven states covering 720 miles with a 6-inch pipe and an 8-inch pipe. It has a pumping capacity of 1180 tons per day.(4) Three releases have been reported on this system in the last 10 years.(1,3) The latest release occurred on July 31, 1981, in the countryside near Willowbrook, KS. An 8-inch pipeline of anhydrous ammonia ruptured at high pressures releasing 700,000 pounds before being stopped by the shut-off valves on both ends. The release occurred in an unpopulated portion of the country and resulted in no deaths or injuries.(1,2,6) The book, High Risk Safety Technology, states that in the event of a catastrophic release of liquefied gas under pressure the chemical may be thrown into the air as a mixture of vapor and very fine liquid droplets. Air may be entrained in the cloud and evaporate the liquid, thus cooling the cloud. This will cause the cloud to act as a dense cloud.(7) Would this have occurred in this case? If so, when would the cloud rise? Would a different model be used for summer and winter conditions? What is the meteorological cut-off point for modeling of this type of release? Do the models consider ammonia leaks that initially act as a dense cloud release, then as a neutrally buoyant cloud, and then as a lighter-than-air cloud?

A third scenario is the release on January 4, 1986, at the Kerr-McGee Corp. uranium processing plant at Gore, OK. A 27,000 pound cylinder of uranium hexafluoride was overfilled by 2000 pounds. In response, employees heated the cylinder to liquify the contents and to remove the material. The cylinder burst, instantaneously releasing 14 tons of uranium hexafluoride, which reacted to form hydrogen fluoride and radioactive uranyl fluoride particles upon release into the atmosphere. The hydrogen fluoride then reacted with the moisture in the air to form toxic hydrofluoric acid. Although the media emphasized the radioactive aspects of the release, the one person killed and the 100-plus injured were attributed to the release of hydrofluoric acid.(8) In this case, hydrogen fluoride has a molecular weight less than air but may act as a dense gas. It may become associated and consist of a mixture of hexamers and monomers with an effective molecular weight of 70. Dissociation takes place as the gas is diluted with air, but the heat required to dissociate cools the mixture and can keep it denser than the surrounding air.(7) Given this scenario, would the hydrogen fluoride form a dense cloud? What models should be used to predict the concentration of hydrofluoric acid under these conditions? Would the models have predicted an 18-mile vapor cloud?(8)

Summary

The purpose of this paper was to answer questions posed by identifying actual case histories and statistics of releases in the United States and to present three scenarios for analysis during the workshop in which it was presented. The scenarios chosen included two of the chemicals most frequently involved in accidents resulting in death or injury (i.e., chlorine and ammonia), and a complex release of hydrogen fluoride.

Table of Conversions

1 mile = 1.6093 km
1 lb = 0.454 kg
1 psi = 6.895 kPa
1 inch = 2.54 cm
$T_f = 1.8 \times T_c + 32$

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SHORT-TERM TOXIC RELEASES FROM CHEMICAL MANUFACTURING SITES

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The U.S. Environmental Protection Agency's Office of Air Quality Planning and Standards in 1985 published in the Federal Register notices of intent to list eight organic pollutants under Section 112 of the Clean Air Act. Inclusion on this list was based primarily on carcinogenic risk potential to the public and, to a lesser extent, on other health effects. Exposure estimates for noncarcinogenic health effects for the intent to list decisions consisted of utilizing information on the continuous emission rates in conjunction with various combinations of terrain and meteorological conditions. An acute risk focus may have resulted in a different group of organic compounds. The eight compounds undergoing evaluation for short-term health effects are:

1. Butadiene
2. Carbon tetrachloride
3. Chloroform
4. Ethylene dichloride
5. Ethylene oxide
6. Methylene chloride
7. Perchloroethylene
8. Trichloroethylene

A program was initiated in 1986 to gather information from processes producing or using one or more of these chemicals to evaluate the potential for noncarcinogenic health effects associated with releases of one or more of the eight organics. The production and related processes considered up to the current time are:

- Butadiene production
- Chlorinated hydrocarbon production
- Chlorinated solvent-using processes
- Chlorofluorocarbon production
- Epichlorohydrin production and user processes
- Ethylene dichloride production
- Ethylene oxide production
- Neoprene production.

This paper summarizes the screening procedure we designed to evaluate nonroutine releases from chemical manufacturing and using source categories. Data are being collected for several types of releases:

- Process vent emissions resulting from start-ups, shutdowns, and control device bypasses
- Pressure relief events
- Equipment opening losses
- Handling and storage emissions
- Accidental releases.

Detailed information to characterize the releases was obtained with a questionnaire. The questionnaires were fairly extensive, asking for information to allow us to pull together the necessary information for submission to our Source Receptor Analysis Branch for modeling.

For process emissions, the questionnaire addresses information associated with start-up, shutdown, or controlled-bypass conditions. Meeting with the Chemical Manufacturer's Association, we received input that helped us to identify those actual process events that result in the higher emissions. There is, of course, a possibility that some events could occur beyond the limits of the profiles that were established, but we are confident that we captured the vast majority of events. Another area where we obtained information concerns pressure relief events. There may be safety relief valves that are designed to automatically relieve overpressure process conditions that may result in relatively high emission rates for short periods.

In the area of equipment openings, the questionnaire inquired about experience and procedures, e.g., in preparing equipment for entry for either maintenance or inspection purposes and where residual material left in the equipment could be released during the procedure. We have found some equipment maintenance activities that represent significant emission sources. Handling and storage of materials also represent a potential source of release. For example, working losses are associated with such activities as pumping into a storage tank. At some facilities, such transfers can involve fairly large vessels. Typical activities include transferring of products to rail cars or tank trucks and the evaporation from wetted material that is not properly sealed.

The final category of nonroutine releases included in the questionnaire involved accidental releases. We have been discussing this category throughout this conference. Examples include failure of a pump seal, liquid spills, and gas or vapor releases.

The data collected via the questionnaire have been used as inputs to a screening procedure to predict ambient concentrations for worst-case conditions. We are working with the Source Receptor Analysis Branch and the Pollutant Assessment Branch of the Office of Air Quality Planning and Standards to combine the information we obtain from the questionnaires along source category lines, as we typically do in our standards development work. For example, for each of the plants that utilize a carbon tetrachloride scrubber on their chlorine tail gas, we are taking the events that have been reported and combining them into what we characterize as a worst-case scenario. Our modelers are also using conservative meteorological and atmospheric stability conditions for evaluating this worst case. If this worst case analysis does not result in a significant health concern, then no further refinements in that analysis are undertaken.

Development of modeling cases incorporating several simultaneous emission events to evaluate potential ambient exposure for a chemical production category is under way, and some preliminary modeling results have been completed. We obtain a plot plan from the source to locate the emission points from the process. Generally, we are looking at averaging times of 15 minutes, 1 hour, and 8 hours, which are typically used for the health effects evaluations being considered. It is also necessary to compare the relative contribution of the various modes of release, i.e., maintenance versus background equipment leaks. If this type of evaluation suggests that health effects may be experienced by the public, then a refined analysis will have to be developed to evaluate short-term releases from the source category.

FATE OF TOXIC RELEASES IN THE ATMOSPHERE--ATMOSPHERIC RELEASE ADVISORY CAPABILITY (ARAC)

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The Atmospheric Release Advisory Capability (ARAC) is an emergency planning, response, and assessment service, developed by the U. S. Departments of Energy and Defense, and focused, thus far, on atmospheric releases of nuclear material. For the past 14 years, ARAC has responded to over 150 accidents, potential accidents, and major exercises. The most notable accident responses have been the COSMOS 954 reentry, the Three Mile Island (TMI-2) accident, the uranium hexafluoride accident at the Kerr-McGee Plant at Gore, OK, and the Chernobyl nuclear reactor accident in the Soviet Union. At this workshop, Joe Knox presented a paper based on the ARAC analysis of the Chernobyl accident. I will discuss the ARAC project in general.

I would like to give you a brief history of the ARAC program. The concept for the project was developed about 16 years ago essentially by three people: Rudy Engleman, now with the National Oceanic and Atmospheric Administration (NOAA) and present here today; Joe Knox, still with ARAC and here today; and Todd Crawford, now with the Savannah River Laboratory. I have had the good fortune to be involved with the project for more than 14 years.

ARAC directly supports the Department of Energy (DOE) and the Department of Defense (DOD) by providing real-time assessments of the consequences that may result from atmospheric release of radioactive

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material. As with any similar program, there are three key components: the staff, the models, and the computer systems. We have a number of meteorologists on the team. Several times during this workshop I have heard comments that meteorologically trained staff are the persons everyone turns to for advice during an accident. The core of the ARAC response team is composed of meteorologists.

The types of incidents that we address are quite varied, and they have numbered approximately 150. They include accidents/incidents in transportation, at DOE facilities, at DOD facilities, at power reactors, extortion threats, satellite reentries, and atmospheric weapon tests. We continue to be involved in a number of tests and exercises for our DOE and DOD facilities and conduct exercises with states and nuclear power plants. As a continuing link to the research community, we participate in planned atmospheric tracer releases.

We serve many masters depending on the type of accident that happens. We serve seven DOE sites (with the potential to serve up to about 15): Livermore National Laboratory and Site 300, Sandia Livermore, Savannah River Laboratory, Pantex, Mound, and Rocky Flats. We directly serve these facilities by maintaining databases for terrain and geography and by having meteorology data coming into our emergency response center in real time. We serve approximately 40 nuclear-capable DOD sites and their commands. During the Three Mile Island stabilization, we worked for both DOE Headquarters and the EPA. We also worked closely with these agencies for the Chernobyl accident. We have worked with several states regarding nuclear material: California, Pennsylvania, New York, Virginia, Florida, and Texas. In fact, we have a fairly broad customer base and during any one incident may work with multiple customers.

While the source term is very important to modeling efforts, one of the first things we learned in the emergency response business is that we will not know the source term at the beginning of an accident. What we do is normalize the source term, which becomes a useful piece of information in our early calculations. Then the people in the field begin to receive data to bracket the effects using the normalized values as multipliers.

In recent years, we have been involved in several toxic chemical releases: a 1976 train accident involving uranium hexafluoride (UF_6), a Titan II accident (even though there was a weapon on board it was not damaged so this was a toxic event because of the missile fuel), a hydrogen sulfide leak during a material transfer at the Savannah River Plant in 1981, the Gore, OK, UF_6 accident, and the white phosphorous rail accident in Miamisburg, OH.

The Miamisburg incident lasted for 5 days, and our colleagues at Mound Laboratory, near the accident, provided input to the evacuation planning process during those days.

The models that we maintain to support our customers must cover widely different scales. For nuclear weapons tests, we have to cover a global scale. As it turned out, we also used global-scale modeling for the Chernobyl event. ARAC's operational models are highlighted as follows.

ARAC OPERATIONAL MODELS FOR NUCLEAR MATERIAL

Model Type	Global Scale =20,000 km	Synoptic Scale =2,000 km	Regional Scale =200 km	Meso Scale =20 km
Simple	--	--	--	Gaussian
Intermediate	2BPUFF	2BPUFF	MATHEW/ ADPIC KDFOC2	MATHEW/ ADPIC KDFOC2
Complex	PATRIC	PATRIC ADPIC	MATHEW/ ADPIC	MATHEW/ ADPIC

MATHEW/ADPIC is a three-dimensional, mass-consistent, wind field model coupled to a particle-in-cell transport, diffusion, and deposition model. It is generally applied to regions 200 by 200 kilometers or less. However, for the Chernobyl accident it was expanded to 2000 by 2000 kilometers. The 2BPUFF is a two-dimensional long-range transport and diffusion model, most often applied to nuclear weapons tests. PATRIC is a three-dimensional, particle-in-cell diffusion model that was specifically designed to treat continental and hemispheric scales; it is a simplified version of the ADPIC model. KDFOC2 is a fallout model used for surface or partially buried nuclear detonations.

These are the models that we have operational. For our on-line sites, where we have databases, we can produce calculations in about 40 to 45 minutes from the time we are notified (new computer capabilities will reduce this time to 15-20 minutes). This is a full three-dimensional calculation. If a site does not have its own capabilities, then we provide them with a system in which they can get simple calculations almost instantly from tower data.

Our regional meteorological data come from the established national meteorological network. For the DOE and DOD sites, the system that remotely collects the data is a DEC PC 350/380. Some sites are connected directly to a local tower with the data coming directly into the system. Others have smaller towers and the data are hand entered. Still others depend on nearby airport data. The minicomputers collect the data, display it locally, and transmit it to the center in Livermore. We also have direct links with Air Force Global Weather Central and a private meteorology company. We receive data from the National Weather Service as well. Thus, we operate a large data collection, database, data analysis, and model-execution facility at Livermore.

We are currently expanding our capabilities in several areas. We are acquiring geographical information from the U.S. Geological Survey for the entire United States. We are currently experimenting with our own local terrain data, including the overlay of model particles on the terrain data. In complex terrain, we are able to overlay the geography, the terrain data, and the particle behavior. Eventually, we hope to be able to accomplish this in real time as part of our normal operational response.

We think some of the high payoff research areas are: 1) development of a local- to regional-scale meteorological forecast model or dynamic model, not for an extremely complex terrain to begin with, but perhaps for rolling terrain; 2) development of a realistic rainout module for both the regional- and global-scale models; 3) continued model evaluation studies; and 4) expansion into toxic chemical response, including addressing the issues of source term, dispersion, and reactivity. The models that we are using today to deal with nuclear releases will be applicable to the toxic chemical events that are nonreactive and at ambient density. We will need to include new capabilities, however, to deal with the chemicals that are reactive and those that are heavier than air. We believe these capabilities should be integrated into the ARAC system in the future as part of a total emergency response capability.

SOURCE STRENGTH MODELING

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Most chemical companies maintain up-to-date material balances around processes in newly designed facilities. They understand what the emissions are and maintain access to models, such as Flowtran^{TM}, (which Monsanto uses) or other similar simulation models to keep the data current.

For the most part, when we talk about process emissions, people normally think of routine emissions. However, I will discuss nonroutine events, such as runaway reactions and fire situations. They will represent elevated sources for which the questions related to dispersion are a lot clearer. Most of the work I will discuss today was done in response to the acrylonitrile standard that the Occupational Safety and Health Administration (OSHA) developed in 1979. Industry attempted to get a handle on whether or not it could meet the objective and criteria OSHA was attempting to address. In response, Monsanto developed a series of models to assist in that understanding. The models were developed in general terms that allow their use with any chemical for which physical and chemical properties are known.

In 1979, Monsanto put its model on-line for any company engineer to use, worldwide, on a computer system over which the developers of the model have no control. The engineers can use it for whatever purpose they wish. While the model has been used for many purposes, most are related to accidents.

Most of the accidents that I will discuss today, relating to releases of organic and inorganic materials, are based on situations such as overfilling tanks or cutting of small pipes. Others have discussed bursting tanks and instantaneous releases today.

Our model best addresses issues dealing with releases where there is a release point, flashing, liquid, and a pool formation. The potential presence of aerosols in the flashing material must also be considered. An engineer, able to use our company model, can usually make a judgment of whether or not an aerosol is involved. We do not know how to model the aerosol yet. The American Institute of Chemical Engineers (AIChE) has initiated some work in an attempt to qualify aerosol behavior. Monsanto's models can, however, handle questions related to flashing, pool evaporation, and release rate.

All of the equations and criteria used in our model are presented in the paper, "Emissions from Spills" by John Wu and me (Air Pollution Control Association [APCA] Specialty Conference, 1979). I will not cover those details today, but will cover other issues. You should understand that the Monsanto emission model can handle different tank configurations, whether they are horizontal or vertical arrangements and whether the structure is a fixed tank or a tank wagon, on rail or on truck. It makes no difference.

In dealing with questions related to diking, the model was designed to deal with the question of how fast the surface of the pool grows. If the release occurs in a diked arrangement, the surface will grow out to a maximum area, and then pool calculations are relatively straightforward. If the material is released into an undiked area, how big will the pool grow? Part of the model and part of the equations presented in our paper deal with that issue. The model will calculate a rate of growth. When dealing with chemicals that volatilize rapidly, such as hydrogen cyanide (HCN), the model will malfunction, because it does not know how to deal with pool shrinkage. The model will reach a point where there is more volatilization than there is incoming material into the pool, and it will fail. However, you can avoid this problem in most cases. By cutting study time back to the time interval that only allows pool growth to the diameter where the amount entering the pool equals the amount evaporating, you can define the critical area. Actually correcting the model is a minor issue that simply requires time.

The question of model validation comes up frequently. One area, of which many of the meteorologists in the audience are aware, is the abundance of pan and lake evaporation data in the world. When we have attempted to match the data for big lakes and ponds, we have found a fairly close comparison.

Our model is dynamic. It solves heat and mass balances simultaneously and provides temperature responses of the pool. Some questions related to cooling arise when dealing with releases of a chemical like ammonia.

A second area, where issues related to source terms come into play, occurs in cases such as spilling material into a sewer or attempting to control a spill by washing it into a waste treatment pond. Randy Freeman and I and a few others have done some work related to surface-aerated ponds and systems using diffused air systems. Short of a long explanation of the models, this requires a steady state model. In this case, we are trying to solve simultaneous differential equations for competitive processes, and we do not know how to do that dynamically yet, at least not with our model and not on a computer system we can afford.

We deal with the question of competitive removal in the model in terms of biological, chemical oxidation, or chemical reaction in competition with air stripping. The user must input a first guess answer to initiate the model. The better the guess, the lower the cost to run the program. The worse the guess, the more expensive it is to run the program. So far, we have done fairly well on closure of the balance. When biological oxidation is going on, you have to have actual information regarding pure material kinetics versus the amount stripped. In the absence of biological oxidation, the model air stripping predictions are within about 3 percent of actual air stripping rates.

In those cases where we must use a "lattice of models," as Dr. Cox discussed earlier, we have the question of what is occurring with respect to seepage into the ground. We have a temperature model that has been built into our "dioxin" model. We refer to the base model in terms of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) only because that is the first chemical we modeled with it. Now, quite a few chemicals have been studied.

The temperature model allows variation of temperature with time at the surface and at different depths within the soil. Behavior of chemicals in the ground has always been messy to profile. The chemical migrates both into and out of the ground. Our focus in using a model for source strength is straightforward, however. We are trying to understand the impact on people by accurately estimating the concentration of the material in the airspace.

Using dioxin, the model was tested with 1984 data from a 1972 Air Force experiment. The dioxin started at about 10 centimeters below the surface and moved up and down. This is unsaturated zone behavior. Dioxin has a vapor pressure of about 10^{-9} millimeters. Additionally, Dr. Nash from the U.S. Department of Agriculture at Beltsville, MD, provided us with data from experiments on dieldrin, heptachlor, and lindane with which we tested the model. Lindane, for example, has a vapor pressure about five orders of magnitude higher than dioxin. If we were looking at benzine or HCN, the same migratory behaviors would be occurring. The only difference is that the migration would not be spread out over 12 to 30 years, it would be over a matter of minutes or hours.

From a safety point of view, the spills model will also model down to something equivalent to TCDD, and we can use it for something that extreme. It does provide conservative values, but does not consider downward migration. Therefore, from the people point of view, if you model only the evaporation from the pool, you have a conservative approach, and that is the central question regarding source terms in active models.

Another source term question area, which we all face, is the runaway reaction question. There you must go to other models, whether it be Sapphire or one of the other models available from AIChE or their contractors. The models available from AIChE and the new ones under development appear to be relatively realistic in providing results. At Monsanto, we use data from an accelerated rate calorimeter to drive a reaction kinetics model for both conditions of runaway reactions and fire impingement on a vessel to determine the rate of release from a rupture disc or a relief valve.

We have heard some about routine emissions in terms of understanding background. We must add fugitive emissions to the list because background makes a difference. If background levels are considered, pool evaporation may be suppressed. Fugitive emissions in the work place have been documented. However, we feel that EPA's work is conservative by a factor of at least ten in a lot of cases for small plants, but realistic for refineries. Fugitive emission estimates provide an idea of the kind of losses that will occur from sources and the impacts that they will have on workers.

Regarding the conservative nature of EPA's estimates of emissions from small plants, we define small plants as those that have small piping and use chemicals of lower volatility than ethylene and propane, which are some of the lighter chemicals found in a gasoline plant. Comparison of actual measured mass emissions from an overall process within a structure versus our estimate versus EPA's estimate will give you an idea of the kinds of ranges available.

There are copies of our paper available, and I would be available to discuss our work with those interested.

FUTURE NEEDS FOR DISPERSION MODELS IN HAZARD EVALUATION, EMERGENCY PREPAREDNESS, AND ACCIDENT PREVENTION

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Someone in the audience observed that there are about 55 dispersion models available at this time, none of which are great and some of which are not any good at all. So, the subject we are dealing with here is certainly very timely. Since this time last year, many events have occurred that have impact on our discussions today. The Chemical Emergency Preparedness Program Interim Guidance has been released in draft form and commented on extensively by the public. It is now being combined with an older Federal Emergency Management Agency (FEMA) document and will be released as the Hazardous Material Emergency Planning Guide. Previously referred to as FEMA-10, the earlier document dealt with contingency planning for hazardous material accidents on a state and local level. The new unified document will be published by the National Response Team and made available through notification in the Federal Register by March 17, 1987.

Recently, a couple of major accidents reminded us that we are dealing with a serious business. The Miamisburg incident caused the evacuation of 40,000 people following a rail accident that released white phosphorous. The Kerr-McGee release of uranium hexafluoride brought an entire new group of facilities into our area of interest, i.e., materials-handling facilities from the nuclear industry. The Kerr-McGee incident also alerted us to areas where we had thought that all government agencies were functioning in a unified way. We learned that there were still some activities that the Department of Energy and the Nuclear Regulatory Commission had not quite aggregated together. This has been corrected, and the Federal agencies now meet on a monthly basis to address issues of common concern regarding accidents specifically.

This year, state and local governments, including the States of Hawaii, Illinois, New Jersey, and California, passed legislation aimed at preparing to provide the public with information on the chemical risks that they face, as well as requiring the state to move forward in preparing for an accident before it occurs. We may even have new Federal legislation in the form of the pending Superfund reauthorization bill. When or if the President signs the bill, it contains an important right-to-know component in Title III.

Basically, it instructs the governors to appoint commissions, who in turn will appoint local planning districts and committees. Those committees would undertake immediate contingency planning around the list of 402 extremely hazardous chemicals (originally published in the Chemical Emergency Preparedness Program Interim Guidance). Facilities that exceed the baseline quantity limits for storage established by EPA must submit information and participate in a broad-based community contingency planning effort. EPA is currently rushing to establish those levels.

If EPA fails to establish another level, the new Superfund bill requires that a base level, i.e., quantity, of 2 pounds be established as the amount of a listed chemical in a facility requiring the submission of contingency planning information. Therefore, two pounds of any one of 402 chemicals will potentially require that a contingency plan be developed for the local community. Certainly, the base level for some chemicals will be increased. However, the important thing is that this will require a contingency plan that will deal with such issues as evacuation, emergency organization, notification, and public health protection. The local committee must include the specific elements of evacuation, identification of hazardous chemicals, identification of the organizations and individuals in charge, and must in fact develop a plan. One of the key issues is going to be what happens when a chemical release takes place? Who makes judgments on how far to evacuate and when? All of these issues are going to depend upon some unified Federal guidance being provided to that local community, in order to assure there is no division, or diversion, or confusion at the state or local levels, as they proceed to comply. Other important aspects of this legislation are that it comes with no Federal funding and that it requires no Federal approval. It says to the governor that it is the state's responsibility and lists several activities the state must undertake to meet that responsibility.

This brings us directly to the issue we are discussing today. The states are going to be clamoring for specific information on modeling. It seems appropriate that the Federal government, in conjunction with public interest groups, industrial associations, technical institutes, scientific groups, and other agencies, can meet together to deal with this issue and to provide state and local governments with information around which they can develop specific contingency plans for those chemicals that are in their community.

There was some skepticism earlier about whether industry would really come forward with the information that would be required to do this contingency planning effectively. The law is going to require that industry not only disclose the existence of the chemical, but also how much they have, and for specific chemicals, where they keep them, and what protective systems exist.

Despite all of this planning, however, a key issue will always remain. That is, what is going to happen when a release occurs in spite of all the precautions that precede, and all the mitigation planning that had occurred? When an event occurs, what is the evacuation route? What is the dispersion probability? What is the plume of the release and what are the effects going to be? It is around these very issues that this and other groups must apply their greatest efforts. It is clear that a lot of dispersion models currently do not take into account issues of topography and weather. When we first sent people to Cameroon, carbon dioxide had not been established as the cause of the deaths, although it soon was. It was a shocking thing to learn that people and all animal life were felled in their tracks 25 kilometers away from a point source by this heavier-than-air chemical. It is hard to grasp that a chemical as common as carbon dioxide could disperse for a distance of some 15 miles and still remain in such intense concentration to kill. Obviously, we have a lot to learn about the dispersion of chemicals in the atmosphere.

We are involved in policy-in-the-making as we work together trying to deal with this problem. Our solutions will provide state and local governments with the ability to respond quickly and accurately for the protection of public health, which is clearly a state and local responsibility. Title III of the Superfund bill is somewhat vague. We will need information on how to set thresholds, add chemicals, or eliminate chemicals; that is certainly within our prerogative. There is, however, no mandatory prevention program included in Title III. While it is not legislatively mandated at this time, EPA is gathering information and reviewing technologies that we think will be able to lead to an improved capability of preventing chemical accidents. While we have a fair amount of activity going on in the prevention area, it is catalytic, not definitive. Most of our efforts deal with prodding others to do their jobs and being sure that there is an adequate transfer of technology.

In this same vein, we believe that dispersion modeling well suits the kind of forum we are having here, where ideas can be shared. In February, 1987, we are having an international symposium in Washington, DC, where the technology that exists throughout the world dealing with the prevention of chemical accidents and the dispersion issue will be brought together. Further, the American Institute of Chemical Engineers (AIChE) is having a major dispersion modeling conference in this country in November, 1987. These kinds of activities are to be commended for supporting the coalescence of information and guidance that can be provided to state and local governments, as they try to make the determinations of how to protect their citizens from future chemical accidents.

We all need to work together, and that is what we are doing. Everybody has a job. The public sector has a job of being a catalyst, a cautious neutral, an informed neutral. The private sector has a job. It is their chemical; their liability. State and local government has a role. They have been responsible for protection of public health and safety on the local level for a long time, and they continue in that role. Federal agencies like FEMA, the Department of Transportation, and the Coast Guard all have a role. Agencies like the Centers for Disease Control and the Poison Control Centers have responsibilities as they review these chemicals and chemical profiles and reach conclusions about how to deal with them. The scientists have a job to continue to move forward in these very complicated technology areas. The citizen has a job, not only a right to know, but a right to become informed. The job requires active participation and learning, not only in assuring that there is a high level of safety, but also in passing appropriate local ordinances where they best prevent chemical accidents from having an impact on people.

Most of all, we all have a job together to try to increase chemical safety in this country. In the event of a chemical accident, we must be sure that the proper information is available for state and local officials who have to make key decisions to protect the public.

ISSUES IN REGULATORY APPLICATIONS OF MODELS

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The Source Receptor Analysis Branch of U.S. EPA's Office of Air Quality Planning and Standards (OAQPS) is responsible for supporting the development of air regulations under the Clean Air Act and, more recently, the Resource Conservation and Recovery Act, as well as supporting activities of other EPA groups in the area of dispersion modeling. OAQPS views modeling needs and issues primarily from the perspective of planning for sudden, unplanned, routine release events, rather than catastrophic releases per se. These issues and needs will be discussed from the standpoint of the following:

- Regulatory and technical background giving rise to the need for dispersion modeling,
- Various technical issues remaining to be resolved, and
- Considerations in devising a framework to approach meeting of those needs.

Although OAQPS is mostly concerned with more routine releases, it is worth mentioning two aspects of planning for the management of catastrophic releases. One is prevention, and the other is emergency response planning. Looking at prevention, specifically as related to hazard analysis (the question of who gets hurt), this is really the place where dispersion models find their best use. Included here are other modeling techniques: source modeling, health assessment, and identification of the release mechanism itself.

Section 112 of the Clean Air Act (CAA) deals with establishing National Emission Standards for Hazardous Air Pollutants (NESHAPS). It requires a listing of hazardous air pollutants first and a setting of standards second. A hazardous air pollutant is defined as one that could cause an increase in mortality or an increase in serious irreversible or incapacitating reversible illness. Thus, from a regulatory perspective, not just situations that cause immediate danger to life, but also those that cause sublethal acute and chronic health effects are to be considered. Section 112 requires that emission standards be set at a level that would provide an ample margin of safety to protect the public health.

OAQPS is currently looking at several types of sudden releases from the standpoint of dispersion modeling. These types of releases may result from:

- Process overpressurization; e.g., pressure relief valve events;
- Transfer and handling operations, e.g., leaks and spills of different magnitudes and sizes and vapor overflow from the filling of large tanks or vessels;
- Malfunction of control devices, e.g., scrubbers and incinerators; and
- Maintenance operations, i.e., typically smaller releases, tank flushing, and equipment opening.

These types of releases have some general characteristics that must be considered. Duration of releases can vary from quasi-instantaneous releases lasting only a few seconds to quasi-steady releases lasting several minutes or longer. There are three depressurization characteristics: 1) rapid jetting action from relief valves and from other pressurized releases, 2) adiabatic expansion and cooling, and 3) two-phase flow. Other characteristics of concern include formation and spreading of liquid pools and evaporation from those pools, along with heating effects associated with the substrate or the atmosphere. Density-related effects include the sinking motion of negatively buoyant elevated plumes, the formation of secondary source clouds with associated dampening of turbulent motion, and the gravity spread of dense gas clouds with terrain contour interaction.

Technical issues of a regulatory nature can be grouped into three basic areas: 1) model selection, 2) model application, and 3) model verification. Model verification should probably be first on this list, but experience shows it tends to be dealt with last.

One of the most important criteria in model selection is the availability of the model in the public domain. For regulatory purposes, proprietary models must generally be excluded. Other aspects related to model acceptability are code standardization and maintenance, and the availability of users manuals and related documentation. The theoretical soundness of the model is also extremely important; i.e., is the model consistent with current knowledge?

Consideration must also be given to whether a model is intended for screening or whether it is a more refined model. Typically, a screening model is both simple and conservative, while a refined model is characterized by being less conservative and more data and computer intensive. One must consider how conservative the screening model should be and how much better an answer is obtained by the more refined models for a given application.

Another important aspect of model selection is the release characteristics that were discussed above, including buoyancy effects, momentum effects, aerosol effects, and reaction effects. A final selection characteristic is terrain, in terms of a generalized surface roughness that affects the rate of dispersion and in terms of specific terrain features that affect wind flow patterns, e.g., upslope flows, drainage winds, and ridge effects. Downslope flows of dense gas clouds may also be an important modeling consideration.

The first issue with respect to model application is the meteorological conditions to be used for the analyses. OAQPS tends to perform two types of applications. First is a screening application where worst case meteorological conditions are used to establish a worst case. Identification of the worst case meteorological conditions generally requires some sensitivity analysis. Second, for more refined applications, a time series of meteorological data is used that reflects autocorrelation inherent in the meteorological data. Questions here are, "What is a reasonable worst case?" and "What is the joint probability that the release event and the meteorological event will occur simultaneously?"

Another issue of model application is averaging time. It would be logical to look at the duration of the release and call that the averaging time, but in modeling, we must be concerned if the emission is varying very rapidly with time. We may need to focus on the period of peak emission. Generally, however, it is the occupational or community exposure standards or criteria that truly dictate the averaging time.

Integration of the source model with the dispersion model is the final issue of model application. As the models and the events to be modeled become more complex, there will be greater need to integrate these two aspects. Of course, there are models available now that do that. Two complex releases, previously mentioned, that may require source modeling in order to specify the initial conditions for the dispersion phase are relief valve discharges and liquid spills.

There are, of course, a number of ways of going about model verification. One can form a theoretical evaluation of a model by simply looking at the model formulation, evaluating it, and evaluating the assumptions of the model on a theoretical basis. Validation of the model code is also important; that is, checking how various numerical techniques in the code are implemented and checking the model code over a range of conditions of the parameters. It is important to adequately validate the model code itself before the model is used. Validation against real data may include both laboratory experiments and field trials. Laboratory experiments tend to be most useful for model development. For verification purposes, their applicability to the real atmosphere may be suspect. In the design of field trials, scale effects (small releases versus large releases), source-related effects, individual chemical effects, and meteorological conditions must all be considered. A very large matrix of field trial experiments is therefore possible, but only a very few are feasible to be actually carried out.

In deciding where to go from here, we must ask ourselves, first, what models do we have that are ready now for regulatory applications, to what situations do these models apply, and with what degree of confidence? Then, we can ask what models have been formulated but are incomplete at this point, to what extent can they be adapted to actual situations, and how can this be accomplished? We must also identify those situations for which no appropriate model exists, whether the absence results from a lack of scientific knowledge or from simply a failure to formalize a mathematical model from existing knowledge, and what can be done to develop the needed models.

In summary, this has been an overview of dispersion modeling needs and issues from the OAQPS perspective in the area of hazard analysis. Some of the issues of model selection, model application, and model verification were discussed, and some suggestions on where we might go from here have been made.

COMMUNITY NEEDS FOR HAZARD EVALUATION TOOLS

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The Environmental Policy Institute, which has been working on the issues of major hazardous accidents for about 6 years, believes that there are now some new opportunities and some new resources that need to come together. Specifically, what can the public sector do within the next 4 or 5 years to improve chemical safety?

A major public problem is that people have not been told what risks they are being exposed to now. There really has not been a communication of potential hazard to the people. Yet, people are going to want to know to what risks and hazards they are exposed. It is fair to say that people in Bhopal were not told of their risks, nor were people at Chernobyl. Certainly, no one in Europe was told that a release event at the Chernobyl facilities could dump its radionuclide inventory on them.

Let me relate a story of how a few months ago I took my 4 and 1/2-year-old daughter to a skating rink in Fairfax County, VA. As we walked up to the rink, I noticed a gigantic petroleum tank farm looming over the rink. Also adjacent to the tank farm are a shopping center and a residential development. I said to myself, "That doesn't look like very smart zoning." Fairfax County is one of the 10 wealthiest counties in the United States and one of the most heavily developing at this time. Obviously, there had been encroachment by the community on an existing tank farm. I decided to approach the local fire chief and inquire about this situation. He reported that this was only one of what he referred to as his "target hazards," and offered to give me what turned out to be a 4-hour tour.

First, we went to an underground propane storage facility. Going into the facility, I knew that this one had leaked. Propane has been found in adjacent creeks. It is good to go to these facilities with the fire chief, because you simply walk in and talk with the operators. A residential community is about 100 yards away from the storage area, separated by only a small fringe of trees. The operator related that when the facility is to be filled, they bring in from three to nine jumbo tank cars simultaneously and fill the cavern. I asked the operator what the community thinks of the facility. He related that several of the people in the community had been told when they were buying their houses that the line of trees was a park where their children could play. In fact, the trees are part of the storage facility. It appeared to me that this was a "Mexico City" accident waiting to happen. Asked why nine tank cars were on site and unloaded simultaneously, the operator related that it took the same time to unload nine as to unload one. Since the people were paid the same overtime, the operator simply chooses to take as many rail tank cars as he receives at one time. It appears that this is an opportunity for some operational improvements to reduce risk.

The fire chief took me to another propane facility, where there were a lot of storage tanks, and where there had been a couple of leaks. He reported that, to get water at the facility, he had to line up fire trucks with over 6000 feet of hose. When he asked the operators to get water to the facility, they refused. It is a preexisting facility and is protected by a grandfather clause from the current safety regulations. The fire chief related several other similar problems. One is a water treatment plant built over 10 years ago with a chlorine facility, but no scrubber. A similar new plant has a scrubber. It appears that a lot of retrofitting is required, and even some fairly simple adjustments in operating procedures would be beneficial.

Part of the problem is that people have not been told what risks they are exposed to. The people of Bhopal and Chernobyl were not told of their risks. There really has not been the communication of hazard to people. In this country, one can illustrate this by looking at the U.S. Department of Transportation (DOT) Emergency Response Guidebook--the "orange book"--that is in every fire truck. There are some "Stone Age," well actually, more "Model T" tools in that book. For example, the phosgene entry says that in case of a spill of phosgene in transportation the fire chief is supposed to evacuate the city 5.2 miles downwind and 3.3 miles wide. There is no fire chief in the country that believes he or she could do that kind of evacuation. Further, there are not 10 city council people in the United States that have ever been told that this material is coming through their city, or that it could require a 17-square-mile evacuation. The guidebook is currently under revision, but that is not the entire message here. There is a basic lack of communication of hazard to people.

People are going to want to know what risks they are exposed to, and, from a community point of view, they are going to need some decent models and some decent techniques to evaluate the risk. These may be either paper and pencil techniques or computerized ones.

At a recent conference at New York University, executives from Johnson and Johnson were talking about their drug case, and Warren Anderson of Union Carbide was talking about Bhopal, when someone in the audience said, "Look, you're describing these major industrial crises from the perspective of a fisherman, rather than the fish." We need to try to look at things the other way around. There is a need for a reversal of the way people look at hazard assessment. It is fair to say that most of the hazard assessment done up to now has been from the perspective of the facility. The facilities have done a lot of hazard assessment already, but little has been done from the perspective of the community. This will be a different perspective, and some simplification will be required. This may be a bit painful for those who have had the resources and the perspective of the facility, and where you want to know exactly what is going on.

The U.S. Department of Housing and Urban Development (HUD) discovered, when they started subsidizing low income housing around the country, that a lot of communities, including Columbia, SC, thought the ideal place to locate subsidized housing for the poor was on what they called "marginal land," meaning right next to the propane facility or right next to the rail yard. The development in Columbia was (to be) right next to (within 150 feet of) 44 propane tanks. HUD did a quick analysis and found that the explosion of just one of those tanks would destroy 60 percent of the proposed 1250 housing units. HUD scrambled and established some "acceptable separation distances" between things that explode and some radius of fire risk, but they still do not even consider toxic clouds. This is the kind of response we can expect. Public safety officials are going to establish various kinds of regulations based on the immediate problems they are faced with.

The National Transportation Safety Board (NTSB) did a rail yard safety study in 1985. They discovered that of eight major rail yards reviewed in the United States, not one of them had an emergency response plan that was coordinated with the local community.

What kind of tools are available to the local community? You can take a 7 and 1/2-minute U.S. Geological Survey (USGS) quadrangle map of any area of the United States, a map of the corresponding city, locate the hazardous facility of interest, and lay down the plume from the NTSB on it. If we use the Miamisburg, OH, chlorine accident as an example, the chlorine would be expected to go 2 miles downwind in 10 minutes at a toxic concentration of 100 parts per million. This is something you can work with, and these are the kind of tools that people are starting to work with now. The city of Denver is doing a rail yard risk assessment right now. After Miamisburg, five cities in Ohio became interested in what was coming through their area.

To many of you who understand the new advances in dense vapor cloud technology, this is going to seem like "Model T" technology. But the fact is that we are going to need something tomorrow, not 2 years or 10 years from now. Local officials are going to need a workable system tomorrow to aid them in hazard assessment, not necessarily quantitative probability analysis. Tools will be needed where normal logic allows you to identify the chemical and the kind of event; then you can identify the consequences and try to engineer solutions.

Some interesting developments are occurring in the United States following the Bhopal incident. Union Carbide came forward with a statement that, "Hey, we ship methyl isocyanate around the United States to five different places much safer than Federal regulations require." They reported that they were using better tank cars, better placards, and special routing to avoid densely populated areas. As a result, the NTSB jumped on DOT, and now they have revised their regulations for methyl isocyanate (MIC) and other similar materials.

It is interesting to note that Union Carbide considers the Federal regulations as minimal. Thus, the better companies have been using far better safety technology than those "minimal Federal codes." We can also lump National Fire Protection Association (NFPA) codes, consensus codes, and other industry codes together. Many of the industries go beyond these, right? What has happened is a lot of "grandfathering". Things have been kept at a minimum level. What we need to do is determine what is the state of the art; what is the best that can be done with a particular technology? Then, when opportunities arise, the regulations can be ratcheted up, so that performance is improved.

In 1985, EPA conducted an inspection of an Allied plant in Baton Rouge, LA, that is using hydrogen fluoride. Allied told the inspectors that they are using state-of-the-art handling of hydrogen fluoride. The inspectors then go down the river to the next facility and learn that that is not state of the art. As a result, Allied must agree to fix things up, and they get a $10,000 fine from the State Department of

Environmental Quality (DEQ). With some sort of public input, there will be some sort of ratcheting up of some of the standards that are not as adequate as others.

The NTSB took the standard chlorine plume and the USGS map of the Potomac rail yard in Washington, DC, and overlaid them. They learned that if the chlorine plume moved east, it would take out National Airport. If the plume moved west, it would take out six schools and a hospital in downtown Alexandria. In the case of the plume moving north, it would take out the Crystal City business complex and the Pentagon. It would seem to be a fair question to ask if the Pentagon or the Crystal City office complex have a system of shutting off incoming air in case of a serious release at the rail complex?

In Middleport, NY, there was a mini-precursor to Bhopal when an FMC facility released some MIC, and it drifted 100 yards to a school. The students started gasping and choking. Since the principal did not have a way to shut off the air ventilation system, he evacuated the students outside into buses that had been waiting to take children on a field trip. They went out into the cloud and were evacuated to a fire station where 200 children had their eyes flushed because of methyl isocyanate poisoning. Now, the principal has a system where pushing a button shuts off the ventilation system, and there is some possibility of sheltering in place. This is the kind of simple solution we must be putting into place.

What are our priorities? What if the public sector is going to have a role? What do we need to do first? This is where we need a lot of help from the experts--those people who have been working in this area for a long time. We need help to identify the kinds of situations that have the most potential. The National Oceanic and Atmospheric Administration (NOAA) developed a real-time emergency response system on an Apple Macintosh computer and placed the system at the Seattle Fire Department for a year's trial. I am very skeptical about this working for emergency response in real time. We may be learning how not to do it. Union Carbide missed the mark with their system during the aldicarb oxime release at Institute, WV. People are going to be developing these real time emergency response systems, whether they are adequate or not.

After Bhopal, we are having a rush to emergency response planning on the part of all the major actors. For example, the Chemical Manufacturers Association (CMA) is touting its Community Awareness and Emergency Response (CEAR) program. CEAR is being implemented in many parts of the country. In the Lake Jackson/Brazosport, TX, area, the CEAR program placed full-page newspaper advertisements about emergency planning. In that area a siren program was developed that covers the entire community with sirens that have a range of one-half mile. A map was provided to the community showing the location of the sirens whose coverage overlapped. When they were asked how the siren locations were selected, they indicated that a map of the industrial facilities was first developed and the location of the major chemicals of concern noted (Map A). Then, the kinds of plumes that might be expected from accidents were mapped, and potentially affected community areas identified (Map B). From this information, locations for sirens (Map C) was established. When asked how the community responded to the map of the potential plumes and effects, the developers of the system responded that they never showed that map to the community. State and local regulators are going to want the whole thing (Map A, Map B, and Map C). They think they have a right to know this type of information.

We have to come up with hazard assessment technology that is workable at the local level and not so refined that it can only be used by a company with $2 million to put into it. We have to have some kind of a hierarchy of hazardous assessment techniques and they have to be acceptable to the local people.

Finally, there is a bit of a double-edged sword in the changes that hazard assessment and emergency response planning are going to precipitate in industry. Union Carbide announced they were using a special transportation planning system (similar to one developed by ALK Associates of Princeton, NJ) for MIC shipments. Union Carbide indicated that special low risk routes are selected and population centers avoided. However, they will not reveal which areas they do go through or what routing technology they use. They know that revealing this information will result in demands being placed on them for other chemicals to be routed with similarly stringent rules. One day before the Bhopal incident, Carbide shipped MIC to five different locations in the United States. One year after Bhopal, there are no MIC shipments in the United States, because people have found safer things to use. This raises all kinds of interesting questions about the potential for safety improvements.

At the AIChE meeting in New Orleans, LA, last year the final session was titled, "Accident Case Histories and Miscellaneous Topics."

At the conference, the session chairman, Dr. Ian Swift, got up and shook his finger at a large audience of engineers and told them that they were going to have to listen to a whole lot of "miscellaneous" papers because "not one accident case history" had been submitted. He said, "I guess your liability lawyers have told you to shut up. This is a very dangerous trend in our industry." It is understandable, but it is dangerous. It is unlikely that the public will think that such an industry has its act together on safety. Bhopal gave them a shock. It is highly probable that there is going to be even more public sector involvement. In Cincinnati, when they passed a right-to-know law, companies submitted 8000 chemicals and declared that all of them were proprietary. The city appointed an advisory board, and now the claims for proprietary information have plummeted from 8000 to 6.

We are going to have a lot of good dialogue between the companies and the public sector in the next few years. We need to work out some workable hazard assessment systems. I am encouraged by the number of people from industry who agree. We need to get to work on the dialogue; it is inevitable.

MATHEMATICAL MODELS FOR ATMOSPHERIC DISPERSION OF HAZARDOUS CHEMICAL GAS RELEASES: AN OVERVIEW

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We need to consider our ability to make reasonable dispersion predictions for use in emergency response. There are two main issues in hazardous chemical (gas) consequence analysis that require the use of atmospheric dispersion models. One is associated with fire and explosions, the other with toxicity. The flammability hazard associated with accidental release of a gas usually disappears when gas has been diluted (with air) to about 1 percent. The toxicity hazard may extend to concentrations four or five orders of magnitude lower. We have spent much more time working on the development of dispersion models for flammable gas concentration problems than we have for toxicity problems.

Analysis of a large number of accidents leads us to consider the important phenomenology in the dispersion process. In releases of large quantities of denser-than-air gases, there will be a part of the process in which the flows are gravity-dominated, i.e., flows driven by the density of the gas rather than the atmospheric wind field. This process is particularly important with flammable gases because considerable dilution sometimes occurs. If we are interested in predicting gas dilution down to 1 percent (the flammable gas issue), these effects are important. However, these processes are much less important if we are trying to predict distances to toxic gas concentration levels. A gas that is heavier than air is stably stratified, and vertical mixing is inhibited. The cloud hugs the ground, spreads laterally, and moves some distance downwind. We are trying to predict the distance traveled before dilution occurs to a given concentration. In the late stages of the event, the dispersion is driven entirely by atmospheric turbulence. We need a model that considers these different phases of dispersion. The model should be able to make a gradual transition starting from the gravitational phase through subsequent phases without the operator having to make the switches.

We have tried to identify the main questions requiring study in dense gas dispersion applications. Our approach has been to isolate different parts of the problem for study. One controversial problem we have addressed occurs with a nearly instantaneous release of a large volume of heavy gas. We know that the gas slumps to the ground and flows out laterally, but no one had (previously) agreed on whether the gas is rapidly diluted during the process. We ran many experiments in the lab involving instantaneous releases of heavy gas volumes, measuring the lateral gravity spreading and dilution. We looked at the scale of the release, the effect of the initial density, and the effect of the initial height-to-diameter ratio of the release. Under these conditions, a heavy gas cloud behaves in an unusual way. Upon release, it rolls up in what has been described as a doughnut or torus formation. Based on the laboratory experiments, we are able to estimate the gravity spreading and the dilution that occurs. Thus, we can now locate the cloud front and estimate peak concentrations that will occur as a function of distance from release.

In the last 10 years, a number of large field-scale experiments on heavy gas dispersion have been completed. At China Lake, CA, the U.S. Department of Energy (DOE) released around 30 cubic meters of liquefied natural gas (LNG) onto water, forming a cloud (visible due to condensed moisture) that moved off downwind. Shell Research, Ltd., conducted similar experiments at Maplin Sands in England. At Maplin Sands, the material was spilled onto water and the dispersion occurred over water; whereas at China Lake, the material was spilled on water and the dispersion occurred over land. The Thorney Island experiments conducted by the British Health and Safety Executive involved the instantaneous release of nominal 2000 cubic-meter gas volumes of heavier-than-air Freon^{TM}-air mixtures. These experiments resemble our laboratory experiments; a container is filled with gas and the container (nearly instantaneously) removed. At Thorney Island, a large tent-like structure was filled with about 2000 cubic meters of test gas, and the side walls of the tent were dropped. The field experiments showed responses similar to the lab-scale ones; the dense gas fell down and rolled up in a doughnut shape. With results of these field experiments corresponding so closely to the laboratory ones, we gained confidence that we can scale our laboratory results to describe field-scale events. We can also take mathematical models that are applicable to a laboratory scale and apply them to a field scale, further demonstrating the scaling relationships derived in the laboratory.

In the last few years, several accidents involving catastrophic releases of hazardous gases have occurred. Considering the liquefied petroleum gas (LPG) terminal disaster in Mexico City in 1984, do we have mathematical models that would give us a reasonable picture of what occurred? I think the answer is yes. Considering the methyl isocyanate release at Bhopal, would application of available models draw a picture consistent with the experience? I think the answer is yes. However, accidents that are difficult to model (even after the fact) have occurred, and consideration of these difficulties leads to identification of areas where additional research is needed.

An accidental release of refrigerated ammonia occurred during a river barge-to-storage tank transfer in Blair, NE, in 1970. Approximately 150 tons of ammonia overflowed onto the tank roof, ran down the tank wall, and evaporated to form a large cloud. Reports of the incident indicated the visible cloud extended 9000 feet from the tank. Because of the prevailing winds, the cloud missed the town of Blair. This is an example of an accident that we do not know how to characterize very well. The release of refrigerated ammonia exhibited all of the characteristics of a heavy gas cloud (the cloud was very wide and shallow and hugged the ground), and it occurred in near-calm conditions.

A high-pressure ammonia pipeline was ruptured by a heavy equipment operator near Enid, OK, several years ago, and a wide plume path, characteristic of a heavy gas cloud was observed. These accidents raise basic questions for which we do not have adequate answers. Ammonia is a material that, because of its molecular weight, would not be expected to form a heavier-than-air gas cloud. Even at the boiling point, saturated ammonia is less dense than air. There was some physical mechanism at work in these two accidents that caused the ammonia clouds formed to be heavier than air. It was probably associated with aerosol formation and evaporation, which cooled the mixture and increased its density. In any case, we have a situation where a heavier-than-air cloud is formed under some release conditions and not under others.

There are two main types of dispersion models: mathematical models and physical (wind tunnel) models. Mathematical models can be subdivided into those using ordinary or partial differential equations. Similarity models (involving ordinary differential equations) are the mathematical models that, in my view, are most appropriate for use in emergency response applications. We assume a regular shape for the cloud, talk about some integrated values that assign the dimensions of that cloud, and calculate how those things develop during the dispersion process. That is, in fact, what Gaussian models do. Three-dimensional mathematical models (involving partial differential equations) can, in principle, simulate the spatial and temporal dispersion process without artificial separation of the flow into separate regimes and may be able to provide for effects of terrain and wake turbulence. Evaluation of three-dimensional models is under way, but most of the work is biased strongly toward evaluation against data for dispersion in the absence of terrain and wake turbulence effects, even though description of these effects is a primary motivation for their use.

DEGADIS (a similarity model we developed for the Coast Guard) distills what we consider the best features of several heavy gas dispersion models. It describes the dispersion of denser-than-air gases on flat terrain and accounts for steady or transient releases. The DEGADIS model, which was based on laboratory-scale experiments and theoretical considerations, has been applied to data from all of the major field-scale tests: the DOE series, the LNG series, the Shell Maplin Sands series, and the Thorney Island series. With these results, a statistical analysis has shown a confidence level with which we can predict the results of these field tests. For all of these field tests, the ratios of observed-to-predicted maximum distance to the 1.0 percent concentration level ranged from 0.88 to 1.33 for a 99 percent confidence interval. In my judgment, this degree of accuracy is good enough for most of the applications we will find in emergency response.

DEGADIS and similar simple models do have shortcomings however. They cannot adequately provide for situations involving obstacles in the flow field, chemical reaction effects, or phase change effects (such as formation of aerosols, evaporation, and rainout). There have been some field tests conducted to address some of these questions. In the Thorney Island tests, some experiments were conducted with (gas) barriers erected around the release site. This particular test was aimed at addressing the situation where a line of trees forms a barrier at the boundary of a hazardous material installation. Simple models also are inadequate in cases where a reactive gas is released. In such cases, one may need to consider the importance of reaction effects. An example is the series of field test releases of nitrogen tetroxide conducted by the Air Force.

For modeling large gas releases on flat terrain, when no important chemical reaction or phase-change effects are involved, we have a number of techniques that are adequate for risk analysis and emergency response application. Future research should be directed to the verification of models that provide for the effects of terrain and wake turbulence and for description of jetting releases, aerosol formation, chemical reaction, and deposition.

Note: This is a summary of the verbatim transcript of Dr. Havens' remarks at the workshop. A complete copy of a paper of the same name, which was presented at the AIChE CCPS International Symposium on Preventing Major Chemical Accidents, February 3-5, 1987, in Washington, DC, appears as Appendix D.

DENSE GAS DISPERSION MODELS

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There have been numerous efforts to model the dispersion of heavy gas releases and most of these have been reviewed in at least one model comparison study or another. Models have been proposed that vary considerably in physical completeness and numerical complexity, and generally, these two model characteristics increase (or decrease) together.

The models that provide the most physically complete description of dense gas dispersion are those that are based on the three-dimensional, time-dependent conservation equations. Examples of this type of model include FEM3, SIGNET, MARIAH, and ZEPHYR. At the intermediate level of completeness and complexity are the similarity-type models. These models use simplified forms of the conservation equations that are obtained by averaging the cloud properties over the crosswind plane. Quasi-three-dimensional solutions are obtained by using similarity profiles, that is, by assuming a crosswind profile for the concentration and other cloud properties. Examples of this type of model include SLAB, HEGADAS, and DEGADIS. At the simplest level are the modified Gaussian plume models. These models are usually used to simulate continuous releases and employ a variety of modifications to include the effects of dense gas dispersion within the Gaussian plume model for trace gas releases. Top-hat models, which are used to simulate instantaneous releases, fall into either the intermediate or

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simple category depending upon the complexity of the model regarding the number of conservation equations to be solved.

In this presentation, a brief description of the representative model types is given with emphasis on the FEM3 and SLAB models being developed at the Lawrence Livermore National Laboratory (LLNL). The details of the various heavy gas dispersion models will not be given here except to point out the main differences between them.

The LLNL has been conducting research for a variety of sponsors in the field of dense gas dispersion in the atmosphere. This research has centered about a number of field-scale test series that were performed in order to gather data to develop and validate dense gas dispersion models. LLNL performed liquefied natural gas (LNG) field tests for the U.S. Department of Energy in 1978 and 1980, and again in 1981 with additional sponsorship by the Gas Research Institute. In 1983, LLNL performed ammonia dispersion tests for the U.S. Coast Guard and The Fertilizer Institute and nitrogen tetroxide spill experiments for the U.S. Air Force. During this same time period, LLNL developed two state-of-the-art atmospheric dispersion models called FEM3 (Chan, 1983; Gresho et al., 1984) and SLAB (Morgan et al., 1983; Ermak and Chan, 1985).

Both of these computer models incorporate mathematical descriptions of the physics of heavy gas dispersion. These include: 1) gravity spread, 2) effect of density stratification on turbulent mixing, and 3) ground heating into the cloud and its effects on density stratification and turbulence. Of the two codes, FEM3 provides the more detailed and complete description of the physics involved in dense gas flows.

FEM3 simulates the dispersion of a released gas by solving the time-dependent, three-dimensional, conservation equations of mass, momentum, energy, and species along with the ideal gas law for the equation of state. In addition, it can treat flow over variable terrain and around obstructions such as cylinders and cubes. Turbulence is treated by using a K-theory submodel. Since it is fully three-dimensional, FEM3 can simulate complicated cloud structures such as: 1) the vortices that are typical of dense gas flows, 2) cloud bifurcation that has been observed during heavy gas releases under stable, low wind speed conditions, and 3) cloud deflection caused by sloping terrain.

The SLAB model solves the crosswind-averaged equations for the conservation of mass, species, momentum, and energy along with additional equations for cloud width and the ideal gas law equation of state. The current version of SLAB also includes the steady-state assumption for continuous releases. Thus, the code is one-dimensional with downwind distance being the independent variable. However, since cloud width and cloud height are also calculated, the model is, in this sense, quasi-three-dimensional. The crosswind concentration distribution is determined by using similarity profiles based on the calculated crosswind height and width. Mixing of the cloud with the ambient atmosphere is treated by using the entrainment concept. The main advantage of the SLAB code is its low computing cost. Typical simulations require only a few seconds on a CDC 7600 computer or a few minutes on an IBM microcomputer.

The various types of models differ considerably in their approach to simulating the atmospheric dispersion of a dense gas release. Perhaps the most obvious differences are related to the degree to which each type of model incorporates the basic conservation laws and three-dimensional effects. The modified Gaussian plume model is based on the single conservation of species equation and either neglects momentum and energy transfer or attempts to include them in some ad hoc manner. On the other hand, the SLAB model includes the conservation equations of mass, momentum, and energy, in addition to the species equation, but only in an average way. Variations in the crosswind plane are neglected, and all properties of the vapor cloud are expressed as crosswind averages that vary in the downwind direction only. The conservation equation model FEM3 includes the most complete description of the conservation laws by treating them explicitly in three dimensions.

A unique feature of the SLAB model is that it calculates only crosswind-averaged properties and characterizes the cloud shape by the height, h, and half-width, B. The parameters B and h do not correspond to any particular concentration level; rather, they can be considered to describe a surface that encloses the bulk of the cloud, for example 90 percent. Consequently, the crosswind concentration distribution is not uniquely defined, making it difficult to compare the predicted cloud shape from this model with the contour plots obtained from the experiments. To overcome this difficulty, one generally assumes a distribution (such as Gaussian, exponential, or quadratic) for the crosswind horizontal and vertical vapor cloud concentration.

There are other important differences related to the manner in which each model treats the effects of gravity and turbulence. As indicated above, the modified Gaussian plume models use ad hoc formulas with "empirical" coefficients to describe the gravity spread and turbulent dispersion of the cloud. In contrast to this, the SLAB and FEM3 models use conservation principles to treat the effects of gravity. This is done in the FEM3 model by solving the three momentum conservation equations, including the buoyancy term and variable density, while the SLAB model solves two layer-averaged momentum equations and uses the hydrostatic approximation.

These two models differ considerably in their approach to turbulence. The SLAB model uses the somewhat artificial concept of entrainment across the cloud-air interface and essentially neglects any explicit treatment of turbulence within the vapor cloud. Air is entrained into the cloud at the surface and then is assumed to mix rapidly in the cloud, creating a nearly uniform layer in the crosswind plane. Thus, there are two separate regions: the cloud and the ambient atmosphere. Mixing between the two is assumed to occur at the interface and is governed by an entrainment velocity that depends on the local properties of both the cloud and the surrounding atmosphere. The FEM3 model assumes that turbulence can be described as a diffusion process and uses a continuous diffusion coefficient that depends on the local properties of the dense gas cloud. While the entrainment and diffusion concepts are peculiar to the SLAB and FEM3 models respectively, the choice of a particular entrainment or diffusion submodel is not an essential aspect of the models. Several submodels have been proposed in the literature and could be used without changing the whole model.

Finally, a three-dimensional, time-dependent, conservation equation model is required in order to describe the distribution of gas concentration in space and time from a heavy gas release into an atmospheric boundary layer with speed and directional wind shear in the presence of complex terrain and man-made structures. The versatility of the three-dimensional conservation equation model in treating more realistic situations and providing a more detailed description of the flow is somewhat balanced by the increased computer costs in running these models. Conversely, similarity models, while giving up some degree of realism and detail, are much faster to run on computers. Consequently, at LLNL we tend to view the three-dimensional conservation equation model more as a research tool that helps us discover new things about the flow, and the intermediate, or similarity model, more as an operational model for situations where computing costs and time are of the essence.

Over the past few years, the predictions from both the FEM3 and SLAB models have been compared with the data obtained from a variety of field-scale experiments. These include the Burro and Coyote series of LNG dispersion experiments and the nitrogen tetroxide spill tests conducted by LLNL and the refrigerated liquid propane tests conducted by Shell Research, Ltd., at Maplin Sands, England. The models have been observed to perform quite satisfactorily within the limits of each model and have been very helpful in identifying the important phenomena associated with dense gas dispersion in the atmosphere.

Basically, three major effects can be observed in the dispersion of dense gas clouds that are not observed in the dispersion of trace emissions. The first effect is a reduction of turbulent mixing within the vapor cloud due to stable stratification of the dense layer. The second is the generation of gravity-spreading and self-induced vortices due to density gradients in the horizontal direction. The third effect, cloud lingering, occurs when the dense gas cloud travels downwind at a slower rate than the ambient wind speed. It is due to a lack of mixing between the dense gas layer and the ambient atmosphere. All of these effects are most pronounced when the ambient wind speed is low and the atmospheric stability conditions are stable.

Perhaps the most dramatic example of these effects was observed in the Burro 8 LNG experiment. In this test, the dispersion cloud developed a distinct bifurcated shape with two lobes on either side of the cloud centerline. This bifurcated structure was due to the combined effects of gravity spreading of the dense gas cloud and a reduction in turbulence allowing this structure to develop without damping out the bifurcated shape. In addition, the vapor cloud lingered over the source region for more than 2 minutes after the spill ended. In all of the other experiments conducted under higher wind speeds and less stable conditions, the cloud drifted downwind from the source within 10 to 15 seconds after the spill had ended. The FEM3 simulation of the Burro 8 experiment simulated both of these effects, namely cloud bifurcation and cloud lingering, quite accurately.

Similarity models have been able to reasonably simulate the average and peak concentration versus downwind distance for the Burro 8 experiment; however, prediction of the cloud structure is beyond the scope of these models because cloud structure is a basic assumption of the models.

One final comment is important regarding the use of dense gas models in operational settings. When an accident occurs, the actual amount of material released and the release rate are often unknown. In order to make dispersion predictions, a unit source simulation is generally performed, and the resultant concentrations are then modified when actual source strength values are obtained. For dense gas flows, the unit source simulation technique is generally inappropriate because of nonlinear effects that are occurring. One cannot simply double the predicted concentration because the measured source strength was found to be double that used in the original calculation. Consequently, this complication of dense gas flows will require a different way of planning for potential accidents.

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ON THE DEVELOPMENT OF REACTIVE, DENSE GAS MODELS

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A summary of this presentation was not prepared at the authors' request. The abstract of a formal paper is given below. The text of this paper can be found in Appendix C.

Chemical reactions between released pollutants and atmospheric constituents can be affected or mechanical turbulence damped. If the reaction is sufficiently exothermic, plume rise can be increased; if sufficiently endothermic, then plume rise can be suppressed. It is necessary to consider the potential influence of such reactions on the mixing rates characteristic of the ambient air. Reaction rates are also a critical issue. If reactions are completed rapidly, then in concept it is possible to assimilate the consequences of the reactions in the source term initialization or in the first time step of a numerical model. On the other hand, if reaction rates are slow in comparison with the time step of a simple model, then a more complicated and detailed modeling effort may be required.

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DISPERSION MODELS FOR NEUTRALLY BUOYANT AND POSITIVELY BUOYANT GASES

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It is my good fortune to be involved with buoyant plume modeling which seems to be much more manageable than reactive and dense gas modeling. I am assigned as a National Oceanic and Atmospheric Administration (NOAA) meteorologist to the Environmental Operations Branch of EPA. Our branch helps to provide a technology transfer link between the research side and the regulatory side of EPA. One of our jobs is to develop, adapt, and evaluate atmospheric dispersion models. These models tend to be operational and not research-grade models like those presented by others at this workshop. We make these models available through the User's Network for Applied Modeling of Air Pollution, which is commonly known by its acronym, UNAMAP.

Since its beginning in 1973, hundreds of people have used UNAMAP either through EPA's UNIVAC computer or through the National Technical Information Service (NTIS), where computer tapes can be purchased. The most recent version of UNAMAP, Version 6, was released in August, 1986, with more than 23 models and programs.

Today, I would like to focus on three programs on UNAMAP that were developed by the Environmental Operations Branch:

- TUPOS - Dispersion estimates using on-site turbulence data
- MPDA - Meteorological processor for dispersion analysis
- INPUFF - Integrated puff model.

TUPOS represents one of the first operational models that incorporated on-site turbulence data. It operates like a routine Gaussian plume model in its steady-state assumptions. TUPOS, therefore, deals only with continuously emitting sources.

In addition to handling on-site turbulence, TUPOS has several other special features. It incorporates layer-by-layer plume rise and partial penetration of a plume into an elevated temperature inversion. It also incorporates recent ideas by Briggs on the modeling of a buoyant plume in a convective boundary layer.

The modeling of partial penetration is particularly important for some sources. Current routinely used Gaussian plume models assume an all-or-nothing approach to plume penetration. If the centerline of the plume is predicted to remain below the elevated inversion, then 100 percent of the plume is estimated to remain in the mixed layer. However, if the centerline is predicted to be above the mixed layer (even by 1 meter), then the entire plume is assumed to loft above the mixed layer. Clearly, partial penetration is an improvement that we feel should be included in Gaussian plume models.

Another important development is the modeling of hesitant or bumping plumes. Willis and Deardorf noted that when a buoyant plume, which is in a convective boundary layer, encounters an elevated inversion, that it can bump against the inversion and spread out laterally. In the Journal of Climate and Applied Meteorology, Briggs discussed a method for predicting diffusion for this situation. The most recent version of TUPOS, Version 2, includes this methodology.

It is hoped that with models like TUPOS we can do a better job of modeling atmospheric pollutants, and certainly there is plenty of room for improvement in this area. If we are to use more complicated models, however, we should have a means for incorporating on-site meteorological data and estimating similarity parameters.

Based on ideas of Irwin, we have developed a meteorological processor for dispersion analysis (MPDA). MPDA allows input of three types of meteorological data: upper-air data from National Weather Service stations, surface observations from National Weather Service stations, and on-site data. MPDA processes all of these data and produces a merged or clean data set. The processor also determines several parameters, such as the solar angle, friction velocities, Monin-Obukhov length, turbulence profiles, and vertical variation of wind speed and wind direction. A great deal of flexibility has been programmed into this model. For many of the parameters, several options are available. For example, there are three options for specifying the sensible heat flux. They are the Irwin-Binkowski scheme, the Holtzlag-van Ulden scheme, and direct determination from on-site turbulence measurements.

INPUFF, developed by Peterson, resulted from EPA's need to evaluate dispersion from incinerator ships. The problem with modeling incinerator ships was that a steady-state Gaussian model could not be used. Therefore, the integrated puff model was developed. In recent years, demand for INPUFF has grown as people have sought programs to model toxic gas releases.

INPUFF simulates individual puffs from one or more sources. Although many sources can be included, the model's speed decreases as the number of time steps increase.

Briefly, INPUFF works in the following manner. At the first time step, a puff is released and disperses according to the specified meteorology for that time step. At the next step, another puff is released so that it and the previous puff disperse according to the new meteorological conditions. INPUFF proceeds in this step-wise manner and is able to calculate contributions at specified receptors from each puff for each time step. Hence its name, the integrated puff model.

Inputs to INPUFF include miscellaneous options, modeling region specification, and source characteristics. Source characteristics include emission rate, time of emission rate, and how the emissions vary with time. Receptor points and meteorological data are included as inputs. Dispersion algorithms included in the model are provisions for initial dispersion, short travel-time dispersion, and long travel-time dispersion.

Currently, the model is designed so that meteorological data are entered for every time step for a user-designed meteorological grid. Eventually we hope that a processor such as MATHEW can be front-loaded into INPUFF to allow a three-dimensional wind field projection.

In reviewing these three programs that are available on UNAMAP, hopefully, I have presented some ideas that may be useful to those involved in the modeling of toxic gas releases.

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LAB-SCALE EXPERIMENTS

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As a physical modeler in a room full of numerical modelers, I must confess I feel like a chicken in a fox house. So, I will do the best I can, and you must decide whether or not you are convinced. I want to talk about the capabilities of physical fluid modeling with respect to meeting the needs of the hazardous materials community. There are many experiments that can be classified as basic fluid mechanics experiments associated with the mixing process. There are tests that have been performed for the meteorological community associated with pre-field test planning experiments. There are concept testing experiments where, for example, a certain mitigation device can be tested for feasibility. There are validation experiments that can be performed specifically to determine whether physical modeling can provide a viable approach to solving some particular problem. Finally, there are experiments that have been directly applied to hazard analysis. The goals of all of these experiments is to test, calibrate, and validate a numerical code.

One might note that if a code is not capable of predicting the behavior of an idealized laboratory-controlled experiment, one should not feel the right or the ability exists to predict a far more chaotic field experiment. As a proponent, I will say a couple of words about the advantages of fluid modeling. Wind/water facilities are in effect

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analog computers, and they have special attributes. They have near-infinitesimal resolution. Grid sizes are not a concern. The transport processes, one could argue, go down to the molecular level. The facilities have near infinite memory. They also have the ability to look at very large three-dimensional grid regions. Fluid modeling incorporates real fluids, not models of fluids. We, therefore, start out using the right stuff in the right place, not someone's concept of how the atmosphere or fluid behaves. Implicitly, this analog computer is nonhydrostatic, non-Bosinnesque, capable of compressible effects, thermal effects, and includes variable property. It includes a non-slip boundary condition, effects of dissipation, and many nonlinear processes. Also, it inherently includes full conservation equations without truncation.

On the down side, there are some limitations. At smaller scales, one must recognize that some similarity is lost in the mixing processes. As speeds drop to handle stratified fluids, the Reynolds numbers decrease, and it is possible that the Reynolds number can drop below some critical value in different phases of the mixing process. Depending on the phenomena, this may result in a minor or a major error. When running experiments at very low speeds, one reaches a point, perhaps associated with the fluid number dominance, where the ratio described as the Peclet number over the Richardson number first proposed by Colenbrander and Puttock from Shell Research, Ltd., is less than some critical value. This means, basically, that you are operating at such a low rate of mixing that the molecular mixing exceeds the scaled turbulent mixing. This is the only phenomenon that tends to give a nonconservative result in physical modeling. Almost all other errors tend to give conservative results.

As smaller scales are used in the laboratory, the separation we are familiar with in the atmosphere between the integral scales, Taylor scales, and Kolmogorof scales of turbulence, will bunch up. Depending on the kind of mixing process under study, this may or may not be important.

There are a number of basic fluid mechanics experiments one might wish to consider. Anyone who has produced a numerical model that uses an entrainment rate at a box-model or a slab-model level or who has worked with various K-theory-type models has probably drawn from physical modeling for basic turbulence coefficients. Some of the earliest work by Lofquist, associated with overflow of fresh water over saltwater, generated the information we use today on the entrainment variation of Richardson numbers. Basic experiments by Kantha, where a surface plate was dragged around and around on top of a circular channel filled with stratified salt water, the merry-go-round experiments, have provided us with additional information. Some errors were later found in these experiments, and meteorologists did experiments to improve this work (Willis and Deardorff and, later, Lindberg). In England, McQuaid has done some basic experiments on transport through dense shear layers associated with carbon dioxide (CO_2) releases. Jerry Havens and I also have done some basic experiments.

We should consider some simple idealized cases. Yang, a student of mine in 1972, and I did some laboratory puff model experiments, where we released thousands of puffs of gas in a boundary layer shear flow and were able to develop models for a transport similarity that included probability density distribution and various coefficients associated with lateral, vertical, and longitudinal variation. These models and the coefficients very closely agree with models we are using today. In 1980-81, Lohmeyer and I did some experiments with instantaneous volumes of dense gases, releasing them at the wall of the boundary layer. At that time, there were no field experiments to guide us, but we identified the basic characteristics of the dense gas cloud. The behavior of the arrival time, the departure time, and the statistical deviations within a multiple sum average condition of a torus-shaped cloud, I believe, are very important. These are critical points for issues of flammability and toxicity. We cannot make decisions based on average conditions, but must know about the statistical range of conditions that exist. A gas cloud is not set on fire by the average conditions that exist. It is the instantaneous concentration that sets the fire.

There have been several somewhat complex studies done in the laboratory, including both dense gas cloud effects and heat transfer effects. The best known of these is the tank experiments on the convective boundary layer concept by Willis and Deardorff. These were heated water experiments that have had a revolutionary effect on both numerical modeling and our field understanding of the convective boundary layer. One of the key points from these experiments is that we now know that clouds released through plumes at the ground tend, in a short distance in a convective boundary layer, to rise. Also, clouds released at elevated points in the convective boundary layer can fall. Maybe on average this point is not so important, but it can make a very big difference in how you should be calculating the results of a toxic or flammable cloud passage.

What kind of pre-field planning experiments are possible? We have performed pre-field tests studying the effects of field terrain, windward variation, and stability. We have looked at instrument placement and cloud extent.

Post-field test experiments also can be useful. Recently in some DOE and Gas Research Institute-funded work preceding the 1987 LGF vapor barrier tests, we found some unexpected things occurred. In the vapor barrier-contained region, we found that the gases sloshed up against the end, hit the barriers like a wave, were caught in the air flow passing over the barriers, and were transported downwind at fair heights. Thus, we found bursts of higher concentrations at higher elevations than were observed in the numerical experiments.

Physical fluid modeling also can play a very useful role in testing of concepts. When the gas industry was looking at alternative secondary containment schemes for large tank storage, there were questions about berm heights for large volumes of cryogenic chemicals. There were questions also about whether soil surfaces or insulated concrete surfaces were better inside the berms and about the comparative effects of these choices on the eventual dispersion of resulting gases. With physical fluid modeling, we were able to test many options and learn not only the answer to those questions, but at that time due to the early nature of those experiments (mid 1970s), we were able to learn new fluid flow fundamentals as well.

In some work with Factory Mutual, funded by the Gas Research Institute (GRI), we looked at water spray curtains and how they mitigate cloud dispersion. In this case, simultaneous field tests were run that were very confusing due to the unexpected results that occurred. Our work on nozzle sizes, varying water pressure, and wind speeds helped to explain the nature and extent of mitigation that did occur in these experiments.

As mentioned earlier, idealized experiments have been used extensively to calibrate modules of various models. Some numerical models have been calibrated against both laboratory and field results. Physical fluid modeling can serve as a useful method for evaluating Federal regulatory-specified accident scenarios at existing or planned facilities. For example, we were able to model such a scenario, a guillotine of a pipeline with 10 minutes of spill at the maximum flow rate, for the Brooklyn Union gas storage facility on Long Island. The experiment showed a positive result, that no effects would be seen beyond the facility boundary in the event of that accident. Since there were resources remaining in the contract, they had us look at larger, even less likely potential accidents, such as spilling the entire tank. This time the results were potentially far more catastrophic, even though unlikely.

Wind tunnel measurements can be very helpful during risk assessment, licensing, or the regulatory process. DOT regulations currently require the use of an extremely over-conservative numerical algorithm. The model does not account for roughness, obstacles, terrain, or mitigation devices. To prepare for licensing hearings for a liquefied natural gas (LNG) peak-shaving facility on Staten Island, we examined spills at about a 1:250 scale model. We introduced conservatism into the experiment by simulating larger, heavier spills in an environment with reduced mixing. The facility appeared to meet DOT requirements even when significantly more extreme conditions were considered than required by DOT regulations.

Recently, field/laboratory validation experiments have been completed for both instantaneous and continuous releases of dense and cryogenic gases. In work for the GRI (Meroney, 1986), I examined some 26 field/laboratory data sets and found that the laboratory-predicted distances to lower flammability limit (LFL) on the average to within 0.4 percent of actual values with a standard deviation of ±22 percent. Pattern comparison plots of concentration isopleths could always be matched by appropriate fluid modeling techniques with less than a 15^0 shift in surface patterns. The British Maritime Technology group in the United Kingdom scaled the recent Thorney Island field spills of Freon^{TM}-air mixtures. They found no apparent lower limit for Reynolds number or Peclet/Richardson number-scaling criteria for collapsing dense clouds.

It is now apparent that fluid modeling can faithfully reproduce the physics of transient dense gas cloud entrainment and motions within the inherent variability of the process for many interesting situations. Fluid modeling can contribute valuable input information for future siting and risk analysis models for the chemical and petroleum industries.

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*Author's/Editor's Note: All of the work by other researchers mentioned in this presentation are referenced in the above citation.

LARGE-SCALE EXPERIMENTS OF THE DOE LIQUEFIED FUELS PROGRAM

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The accidental release of hazardous gases into the environment often results in what has come to be known as dense gas behavior, even when the gases themselves may be nominally less dense than the atmosphere into which they are released. This dense gas behavior can dominate the consequences of the accidental release making it either worse or better than might otherwise be expected and making prediction of the consequences of the release difficult. There are a number of contributing causes of dense gas behavior, including large-scale release, low temperature, flashing, chemical reactions, evaporative cooling, and molecular weight. Cloud behavior differences are due to density or gravity-induced effects (turbulence damping); thermodynamic effects (aerosol formation and flash vaporization upon release, evaporative cooling, or heat transfer from the ground modifying cloud buoyancy and turbulence); and chemical reaction effects (hydrolysis with atmospheric water vapor, polymerization, or decomposition, which also affects cloud density). These effects are very important close to the release point, but also can have dramatic effects on the cloud as it disperses downwind.

The study of atmospheric dispersion of dense gases began as a new scientific field in the 1970s. Interest was prompted by a series of accidents: Flixborough in 1974, Seveso in 1976, and the Houston ammonia accident also in 1976. The interest in this field has always been more intense in Europe than in the United States. As a result, much of the research has been done in Europe. Early work in the United States centered around liquefied natural gas (LNG) safety, and this was when Lawrence Livermore National Laboratory (LLNL) got involved, starting in 1976. Many people at this conference got involved at about this same time with the LNG safety program.

Work on dense gas dispersion continues to involve three complementary areas:

- Mathematical modeling based on physical laws
- Near full-scale field experiments to:
    1) Discover unknown and important effects in scaling laws
    2) Simulate accidents or evaluate mitigation equipment
    3) Validate models
- Scaled-down simulations in the laboratory, wind tunnel, or water flume.

We have discussed all of these at this workshop except large-scale experiments on which I will focus my remarks.

There have been a number of recent large-scale field tests with dense gases. I will focus on the most recent and the best instrumented. These are the tests that are currently being used in developing databases for model comparisons and model validation. Most of the good quality data have been obtained since 1980 when, essentially simultaneously, Shell/NMI conducted a series of LNG and liquefied petroleum gas (LPG) trials at Maplin Sands in England, and DOE/LLNL conducted the Burro series of LNG tests at China Lake, CA. These tests resulted in the discovery of previously unknown and important effects. The Maplin Sands tests involved spills of about 5 to 25 cubic meters of LNG with spill rates between instantaneous and 1 to 5 cubic meters per minute. DOE's Burro series, conducted at about the same time, focused on dense gas dispersion and involved spills of 24 to 39 cubic meters at rates of 12 to 18 cubic meters per minute. A follow-up series of DOE tests conducted in 1981 was called Coyote. These tests were designed to get information on three different areas: combustion, dispersion, and rapid-phase transition explosions.

There are a number of reasons for doing field-scale experiments. Many of the effects that occur upon accidental release of dense gases are poorly understood. In some cases, the effects have been observed in the laboratory, but the extent of what will occur or what will be important or dominant in accidental releases is unknown. The important physical effects in dense gas dispersion include:

- Gravity spreading
  - Low cloud
  - Displaced ambient wind field
  - Self-induced vortices
  - Increased surface area
  - Increased wind shear
  - Increased heat transfer
- Turbulence damping
  - Stable stratification
  - Impenetrable interface
  - Negative turbulent mass flux
  - Evaporating droplets
- Heat transfer
  - Increased ground contact
  - Decreased air entrainment
  - Enhanced evaporation and condensation for cryogenics spilled on water
  - Chemical reactions with water vapor or other species
- Turbulent entrainment
  - Turbulence generated by the release (internal)
  - Atmospheric turbulence excluded
  - Heat transfer generates convective cells
  - Jet releases entrain air
  - Instabilities

Additionally, much of the physics dominant in dense gas dispersion is highly nonlinear and, therefore, not easily scaled to larger size. Very stable atmospheric situations and nonisothermal (i.e., heat transfer, condensation, etc.) effects can often be important and are also not easily scaled. In many cases, dominant behavior at large scale was not even observed in small-scale tests. For instance, dense gas behavior is not observed for small releases in the atmosphere; turbulent dispersion dominates. Thus, two of the major reasons for performing these tests are the discovery of unknown and important effects and determination of their scaling laws. These well-instrumented tests allow quantitative measurement of these effects so that correct descriptions can be incorporated into the mathematical dispersion models. This is necessary if accurate predictions are to be made for circumstances different than those under which tests were performed. As you can readily see, dense gas dispersion is very complicated.

Other reasons for conducting field tests include accident simulation or evaluation of mitigation equipment such as water or steam curtains. These can be situations that are simply too complicated, with too many unknown contributions to yield to mathematical or physical model simulation. Other complicating effects that are difficult to model or scale include chemical reactions and certain non-reversible thermodynamic effects, such as flashing, two-phase flow.

Perhaps the most common reason to conduct large field experiments has been to obtain basic data for dispersion model validation. This requires extensive, carefully verified, quantitative data from well-documented and well-instrumented experiments. The need for such data was demonstrated by McQuaid of the British Health and Safety Executive, in 1983 when he invited the mathematical modeling community to predict in advance the results of an instantaneous release of 200 cubic meters of gas with an initial density two times that of air. Variations between models of two orders of magnitude were present even for this relatively small, isothermal release onto flat terrain without chemical reactions, thermodynamic effects, or other complications. Models have improved since that time, but the tasks we are giving them are much more difficult and include many more complicated effects. Thus, model validation continues to be one of the major reasons to conduct field experiments. In spite of the number of tests that have been conducted, data for model validation are still in short supply.

There are many difficulties associated with the conduct of large-scale field tests. They involve huge instrument arrays with hundreds of individual instruments and their attendant maintenance and calibration. These extensive arrays are necessary because gas cloud behavior is highly variable in space and time and complicated by the presence of the many simultaneous and interactive effects mentioned earlier.

The large-scale, well-instrumented spill tests that have been conducted since the 1970s have contributed much to our understanding of dense gas dispersion. Dense gas characteristics are particularly important for large releases, low wind speed releases, stable atmospheric conditions, low-level inversions, and proximity to the release point. Proximity to the release point is very important for dense gas releases. In our ammonia release tests, we were still measuring dense gas effects at a distance of 3 kilometers. Dense gas behavior is caused by large size, low temperature, flashing two-phase flow, chemical reactions, evaporative cooling, and molecular weight. Many of these effects are nonlinear, and, therefore, it is important to base calculations and predictions on size.

Not all of the things that people do can be scaled, depending on which dominant effects are of interest. Dense gas releases exclude ambient atmospheric processes. Gravity spreading and turbulence damping decrease dispersion, while heat transfer and turbulent entrainment can increase it. Dense gas effects do have profound influence on our ability to predict the consequences of accidental releases.

In summary, there are a number of reasons for doing field-scale experiments. Many of the effects that occur upon accidental release are poorly understood. In some cases, they have been observed in the laboratory, but the extent of what will occur or what will be important or dominant is unknown. In addition, much of the physics dominant in dense gas dispersion is highly nonlinear and, therefore, not easily scaled to larger size. Thus, two of the major reasons for performing these tests are the discovery of unknown and important effects and determination of their scaling laws. Well-instrumented tests allow quantitative measurement of these effects so that correct descriptions can be incorporated into the mathematical dispersion models. Models are necessary if accurate predictions are to be made for circumstances different than those under which tests were performed. Other reasons for conducting field tests include accident simulation or evaluation of mitigation equipment such as water or steam curtains. These can be situations that are simply too complicated, with too may unknown contributions, to yield to mathematical or physical model simulation. Other complicating effects that are difficult to model or scale include chemical reactions and certain nonreversible thermodynamic effects such as flashing two-phased flow. Perhaps the most common reason to conduct field experiments has been to obtain basic data for dispersion model validation. Today's sophisticated models require extensive, carefully verified, quantitative data from well-documented and well-instrumented experiments.

FLUID MODELING OF DENSE GAS DISPERSION OVER A RAMP

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Recently, we completed our first foray into dense gas dispersion at the U.S. EPA Fluid Modeling Facility at Research Triangle Park, NC. Rex Britter from the University of Cambridge drew up the plans for the first research study. Unfortunately, he could not be here to present the work today.

We have drawn upon our previous experiences in modeling and simulating dispersion in the neutral atmospheric boundary layer. This work has focused mostly on ground-level and elevated point sources. We have also done numerous studies in the wind tunnel on the flow structure and dispersion around isolated hills of simple geometry and studies in the towing tank of flow structure over and dispersion of plumes within stratified flow over isolated hills. The new addition to these programs is our subject today, dense gas.

One of the biggest problems we have encountered was alluded to today by Bob Meroney. That is the fact that when you simulate a plume that has a density different from that of its environment, you need to do Froude number scaling, which means you need to reduce the wind speed. By reducing both the scale and the wind speed, you have reduced the Reynolds number, which means that what would have been a turbulent flow in the wind tunnel may now become a laminar flow, irrespective of the density difference. In addition, if you are modeling a positively

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buoyant plume, i.e., a destabilizing influence, you may be able to model that at a smaller-than-normal Reynolds number. However, in the case of a dense gas plume, the dense gas has a stabilizing influence. This stabilizing influence of the density gradient plus the reduced wind speed due to the Reynolds number makes the simulation of dense gas dispersion in the wind tunnel doubly difficult.

Our first exercise in the wind tunnel was thus a flow-visualization study. We used carbon dioxide (CO_2) as the effluent in a wind tunnel boundary layer, which had previously been used for point source studies. We fixed the mass flux of CO_2 at the rate planned for later quantitative studies. Smoke was injected in order to be able to see the plume. We visualized the plume in the tunnel at various wind speeds, watched the plume to see that it remained turbulent, and progressively reduced wind speeds until the flow became laminar. We found that the plume remained fully turbulent to wind speeds as low as 1.0 meters per second. Thus, we selected this wind speed for the remaining quantitative tests. We have prepared a videotape of these flow visualization tests.

Our source configuration consisted of a metal can filled with gravel up to the level of the tunnel floor to maintain a homogeneous flat surface across the source. The CO_2 was emitted through the gravel, and was thus emitted in a circular area through the flat surface. We placed a honeycomb at the entrance of the test section of the wind tunnel to stabilize the flow. A straight fence served as a trip to generate a simulated neutral atmospheric boundary layer. From previous experiments, we knew that this was a reasonably well-developed boundary layer. The source was placed about 8 meters downstream of the fence.

For an initial series of tests, we emitted CO_2 and/or air from the source and then measured the detailed structure of the plume downstream in longitudinal, vertical, and crosswind or lateral concentration profiles. Later a ramp was included in one of two positions either 1800 millimeters downstream from the source or 600 millimeters downstream from the source.

Looking at the boundary layer structure of these experiments, we found that for mean velocity profiles between 1 and 4 meters per second, the flow is virtually independent of Reynolds number. Longitudinal turbulence intensity profiles also show that structure to be virtually Reynolds-number independent.

For the quantitative portion of the study, about 3 percent ethane was added to the source, so that concentrations could be measured downstream. These measurements, again, show that at 1 and 4 meters per second the concentration and dispersion field in the wind tunnel were independent of Reynolds number. Much additional data on the flow structure are available due to this and previous work. There are hot-wire anemometer measurements of mean velocity profiles, flow angle, longitudinal fluctuating velocities, and other parameters.

Streamline patterns derived from mean velocity profiles show divergence of the flow from upstream to the base of the ramp, followed by convergence of the flow from the base to the top, and a slight divergence downstream from there.

Using CO_2 (52 percent heavier than air) with smoke added for visibility, we have demonstrated that for flat terrain with free stream wind speeds of 2 and 4 meters per second, plume buoyancy is unimportant. However, at lower wind speeds, strong lateral spreading of the dense plumes was observed. Thus, we conclude that under these conditions, a significant buoyancy effect exists.

Repeating the above experiments with a ramp placed 1800 millimeters downstream of the source, a significant widening of the plume is seen both in the neutral plume case and in the dense plume case. When the wind speed was reduced to 0.75 meters per second, laminarization of the plume was observed. At 0.5 meters per second wind speed, obvious streaks, indicating laminar behavior, were observed. We do not believe that a valid model of a full-scale problem is achieved when laminarization occurs.

To compare the dense gas plume with the neutral plume, we plotted the concentration normalized by the source concentration as a function of downstream distance. The decay of the centerline concentration with downstream distance in the dense plume is essentially identical to that of the neutral plume. The model scale ratio used was approximately 1000 to 1. Far downstream, the slope is about -1.5, typical of the downstream behavior of a point source in a neutral atmospheric boundary layer. Closer to the source, the slope is -1.0, which has to do with the finite width or area source. Thus, in spite of the differences in the plumes observed visually, the centerline ground-level concentration patterns changed very little. Therefore, this is not a good indicator in field measurements of whether a dense gas plume or a neutral gas plume has been released.

In our studies, lateral concentration profiles of the plumes were measured at 300, 600, 1800, 5000, and 8500 millimeters downstream. Gaussian distributions were extremely well fitted to the lateral concentration profiles of the neutrally buoyant plumes. Dense gas crosswind lateral profiles are not Gaussian at all; they are essentially flat topped.

The centerline concentrations for the dense gas and neutral gas plumes are essentially identical. However, vertical concentration profiles differ dramatically. At the 50-millimeter elevation, the concentration for the neutral gas plume at 300 millimeters downstream is about 50 percent of the surface concentration. In the dense gas plume, the concentration at the 50-millimeter elevation is more than two orders of magnitude lower than the surface concentration value. Farther downstream, the dense plume tends more toward neutral or well mixed at the surface.

In our experiments, the dense gas plume starts out substantially wider than the neutral plume due to lateral spreading right at the source. The dense gas issuing from the source actually creeps upstream approximately one half of a source diameter. A very short distance downstream, the lateral growth rates of the neutral and dense gas plumes are essentially identical, i.e., equal slopes of the curves.

Comparing the centroids of the two distributions, a measure of the vertical widths of the plumes, the negative buoyancy appears to be significant as far downstream as you choose to compare.

Looking at ground-level concentrations of the neutral gas plume as a function of downstream distance on the centerline with the ramp installed, the ramp induces a ground-level reduction of approximately 20 percent. This is not a major difference. With the dense gas plume, the ramp induced perhaps a 20- or 30-percent decrease in ground-level concentration.

Anticipating that the buoyancy would be more important closer to the source, we moved the ramp closer to the source. In that case, the ramp induces perhaps a 30- to 40-percent reduction in ground-level concentration for the neutral plume. With the dense plume, the ramp induces about a 50 percent reduction in concentration at ground level.

An extensive experimental data set on the detailed structure of a dense gas plume resulted from these studies. The model depicts a dense gas plume that has significant buoyancy effects, but which, nevertheless, will be insignificantly affected by molecular effects. Data also were collected for the neutral plume in the same experimental setting to support comparative analysis.

In summary, the longitudinal centerline concentration profiles of the dense gas plume were strikingly similar to those of the neutral plume. However, plume shapes were dramatically different; the dense plume being much wider in the lateral direction and much narrower vertically. Lateral distributions of the dense gas plume were top-hat shaped, essentially uniform all the way to the edges. In contrast, lateral distributions for the neutral plume were essentially Gaussian in shape. Introduction of a ramp into the experiment induced a slight reduction (20 to 30 percent) in the ground-level concentration when the ramp was far downstream. When the ramp was located close to the source, the reductions were somewhat greater. Reductions were also somewhat greater for the dense plumes than for the neutral plumes, but not significantly so.

ATMOSPHERIC SCIENCE AND EMERGENCY RESPONSE AT THE SAVANNAH RIVER LABORATORY

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The Savannah River Plant (SRP) is a nuclear production facility owned by the U.S. government and operated by du Pont. SRP is located in South Carolina on the Georgia border near Aiken, SC. It is the third largest nuclear materials production site of the Department of Energy (DOE) and includes nuclear fuel production, fabrication, irradiation, and reprocessing. A program for responding to unplanned releases into the atmospheric or aqueous environment of radioactive toxic chemicals is essential, and one has been in place since the facility began operation in 1953. There has been an atmospheric dispersion research program at SRP for almost 15 years. The consolidation of emergency response and atmospheric research has strengthened both programs.

The SRP encompasses 315 square miles of mostly wooded, gently rolling terrain. Four operational reactors, two chemical reprocessing plants with high-level waste tank farms, a tritium processing and handling facility, and a fuel fabrication facility are operating. A waste vitrification facility and a naval fuels fabrication facility are under construction. Hazardous effluents that accidentally could be released into the atmosphere from these facilities include tritium (elemental and oxide forms), gamma-emitting aerosols, radioiodine,

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transuranic aerosols, radioactive noble gases, and chlorine gas. The Savannah River runs across the southern border of the plant.

The Environmental Transport Group (ETG) is charged with characterizing and calculating the transport and dispersion of atmospheric and aqueous releases from SRP facilities. The group is composed of 14 professionals and 8 technicians, including 5 meteorologists, an oceanographer, 2 health physicists, a nuclear chemist, and a computer systems manager. At least two meteorologists and a supervisor are on call for emergencies. Pertinent information is reported to DOE and du Pont managers for final action. Environmental impact and regulatory document matters are assigned to a separate group although ETG offers expert assistance as needed.

The primary aim of emergency response activities at SRP is to quickly identify and characterize any accidental release of materials and to provide SRP decision makers with the information necessary to respond wisely. The emergency response system has two major components, the WIND system and the TRAC mobile laboratory. The Weather INformation and Display (WIND) system is used for data acquisition, archiving, and model calculations. Data enter the WIND system from the Remote Environmental Monitoring System that provides:

- Real-time wind and turbulence data collected from 8 single-instrument, 60-meter on-site towers and a nearby 300-meter television tower instrumented at 7 levels;
- Regional meteorological data from the Automated Field Operations Services (AFOS) system;
- Data from temperature monitors in on-plant streams and the Savannah River;
- Real-time source term information from stack monitors; and

- Real-time plant boundary radioactivity measurements from perimeter monitors.

The WIND system utilizes VAX 780 and 750 computers to process these data, run dispersion models, and support remote terminals in each operating area. The TRAC mobile laboratory is used for plume tracking and real-time radioactive monitoring. These systems are operational 24 hours per day, 365 days per year.

The research programs at SRP emphasize mesoscale atmospheric dispersion. The present field program, Mesoscale Atmospheric Transport Studies (MATS), is designed to determine the accuracy of dispersion and transport models and to measure horizontal plume width. The downwind distance range of greatest current interest is approximately 30 kilometers, which coincides with the major population centers surrounding SRP, Augusta, GA, and Aiken and Barnwell, SC. Since 1983, this program has been concerned primarily with measurements in unstable atmospheric conditions, but this year the emphasis has shifted to measurements in stable conditions. The experiments simulate short (15 minutes), intense puff releases. A sulphur-hexafluoride (SF-6) tracer is measured downwind from a 60-meter stack with fixed, sequential samplers and a mobile, continuous sampler in the TRAC vehicle. The fixed samplers are deployed by many of the same team workers who are called during actual emergencies. Sampling in the TRAC vehicle is done to measure the instantaneous horizontal puff width during passage over the 30-kilometer arc. To date, 26 daytime experiments and 3 nighttime experiments have been completed in the MATS program. An additional 25 nighttime and several more daytime experiments will be completed in the coming year.

A spin-off from the MATS program is the STable Atmospheric Boundary Layer Experiment (STABLE). The objective of STABLE is to develop an understanding of turbulence and dispersion at mesoscale range in the stable (nocturnal) boundary layer and to improve the models for dispersion under these conditions. It is expected that the largest offsite doses would occur from a release in stable conditions. STABLE will include study of a 5-year turbulence database, interlaboratory field experiments, and extensive model evaluation and development. The fact that both the Bhopal and Chernobyl accidents occurred during stable nighttime conditions has given additional impetus to this program.

The consolidation of operational emergency response and research programs in one medium-sized group with a single group manager has greatly benefitted both programs. Researchers can utilize the laboratory and technical abilities of carefully trained emergency response specialists. On the other hand, emergency response personnel learn the latest observational procedures while gathering data for research applications. Moreover, dispersion and transport codes are tested and improved using results from research. Finally, operational feasibility of research results can be tested during emergency response exercises.

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EMERGENCY PREPAREDNESS AND RESPONSE IN THE U.S. AIR FORCE

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The U.S. Air Force Engineering and Services Center, where I am assigned, is designated as the focal point within the Air Force for environmental quality research and development (R and D). While we do not do all of the R and D work, we do try to keep up with what is happening in this area. When we recognize a need for research, we are responsible for initiating a project to fill that need. We also are responsible for coordination of research activities with other agencies within the Air Force and the Department of Defense, such as Headquarters, Air Weather Service, and Air Force Geophysics Laboratory. We identify needs in the field and try to develop tools that people in the operational areas can use to prevent an adverse impact on the environment.

With regard to emergency response, the Air Force is interested, basically, in two kinds of events--hot spills and cold spills. In more technical terms, a hot spill refers to any event involving a fire or an explosion, while a cold spill does not. That terminology comes from the people actually working in the field in missile range safety and at various missile sites. A fire or explosion generally involves some type of missile explosion, either the vehicle itself or the stored propellants used to fuel that vehicle. Cold spills may involve a release of liquid missile propellant or a release of aircraft fuel, but do not involve fire or explosion.

Focusing on hot spills, we are primarily concerned with two types of propellants. Both the liquid and solid propellants are toxic. The primary liquid propellants are nitrogen tetroxide (N_2O_4) and Aerozine-50 (A50), a 50:50 mixture, by weight, of hydrazine and unsymmetrical dimethylhydrazine (UDMH). Both of these are very toxic and, because they are stored in liquid form, are mobile in the environment when spilled. The typical solid propellant in the Air Force is composed of ammonium perchlorate and aluminum. The primary combustion material resulting from the ammonium perchlorate-aluminum mixture is hydrogen chloride, which, when compared with N_2O_4 and A50, is not very toxic. However, we must be concerned with local and climatological effects of a large hot spill of the solid propellants. We must also consider the situation of a hot spill with both types of propellants. For example, when the Titan 34-D blew up shortly after liftoff at Vandenberg earlier this year, both liquid and solid propellants were involved.

A typical explosion involves a fireball that lifts, stabilizes at a certain height, and then disperses. At the two largest launch sites, Vandenberg Air Force Base and Kennedy Space Center, meteorological data available at the time of the accident are extensive. There are a large number of towers. Vandenberg currently has 26 towers on the reservation. These towers are instrumented at various heights, have instruments for mean wind speed and direction and temperature, and can measure temperature differences at various heights to get an idea of atmospheric stability. We also directly measure the standard deviation of wind direction at various levels. Prior to launch at these locations, a rawinsonde run is made to gather further information about the stability characteristics of the atmosphere, particularly at higher altitudes.

At other sites, primarily Intercontinental Ballistic Missile (ICBM) sites, instruments are much less numerous. At these ICBM sites, we have the capability to get mean wind speed and direction at approximately 10 meters above the ground. Also, we have the capability to estimate the standard deviation in wind direction and determine a value for the vertical change in temperature. That value for the vertical change in temperature is the primary means that the Air Force currently uses to characterize atmospheric stability.

The tools we have for modeling a hot spill are currently limited. The Hypergolic Accidental Release Model (HARM) was developed specifically for the Titan II missile system that is fueled with hypergolic liquid propellants. The Rocket Exhaust Effluent Dispersion Model (REEDM) was designed to estimate the ground-level concentrations of gaseous hydrogen chloride resulting from a Space Shuttle launch. REEDM is used primarily for planning prior to a Shuttle launch; however, it does have a module to handle a launch abort or explosion, which would release fairly large quantities of hydrogen chloride.

The primary meteorological input to HARM is rawinsonde data. HARM has a preprocessor that calculates the source term taking into account the heat released by varying amounts of hypergolic liquids. It calculates an initial fireball size and cloud rise, and the resulting dispersion is modeled using a Gaussian puff model. There is an algorithm that estimates the amount of deposition due to rainout. The primary outputs of the model are ground-level concentrations of the combustion products of interest.

The role of the meteorologist in these hot spills depends on where the accident occurs. At Kennedy and Vandenberg, a meteorologist is heavily involved in planning and in responding to accidents. The REEDM model is run by the meteorologists and is used extensively for risk assessment. Risk assessment is generally done well in advance of a launch and involves a large number of computer runs using climatology to determine a worst case scenario. REEDM is used for planning just prior to a launch using forecast winds and temperatures. It is used for accident response as required; but there really is limited time and many more things to worry about than running a model immediately after an accident.

At other locations, such as the ICBM sites, the meteorologist's role is less well-defined and tends to be up to the local commander. For risk assessment and for planning and response, the heaviest involvement is with the safety and operations personnel. This is principally a condition of geography. The meteorologist is not at the missile site that has a problem. He or she is at a central location, and it is the on-site people that must do the planning and response. However, the meteorologist is involved in post-accident analyses.

There are two broad areas of interest with respect to the Air Force's response to cold spills: 1) a spill involving Air Force materials and occurring on Air Force property or 2) a spill involving industrial chemicals occurring off of Air Force property. The latter category is included because the Air Force is obligated to assist if an accident occurs near an Air Force installation and the local authorities asked for assistance. As a result, the Air Force meteorologist occasionally gets involved with calculating toxic corridors for non-Air Force materials and non-Air Force locations.

On Air Force property, our primary concerns are the missile propellants, N_2O_4 and A50, and other types of hydrazines used in various aircraft. There are also relatively small quantities of typical industrial chemicals on Air Force installations, such as chlorine, which is used in water treatment plants.

Cold spills do sometimes occur in missile operations. For example, in 1978, a Titan II site in Kansas experienced a N_2O_4 spill. In such cases, the meteorological information available depends upon the site. Kennedy and Vandenberg are, again, well instrumented. At the missile sites, such as Titan II and Miniteman sites in the Midwest, meteorological information is relatively limited, but they will have, at a minimum, wind speed, direction, and the vertical change in temperature. At a typical Air Force base, not supporting missiles, but experiencing a hydrazine spill from an F-16 aircraft, the only meteorological information available is usually mean wind speed and direction, temperature at a height of about 6 feet above the ground, and a very rough means of estimating the vertical temperature profile and the standard deviation of wind direction. If a spill occurs near Air Force property, but not on it, the amount and quality of information available is highly variable and, typically, very limited. Off base, the information available typically depends on the proximity to the base or to a National Weather Service site.

For cold spills, there are a few models that we have available. One is the well known Ocean Breeze/Dry Gulch (OB/DG) equation, which has been available since the mid-sixties. This is an empirical equation derived from a large number of tracer releases. It was developed by the Air Force Geophysics Laboratory. There are several other similar equations that are not as well known, such as the Mountain Iron and Sudden Ranch equations, which are used at Vandenberg primarily. These are based on a series of releases of material at a specific location and are used only at that location. Vandenberg is an interesting and complex place meteorologically. Vandenberg is in a coastal situation approximately 150 miles northwest of Los Angeles; therefore, it has coastal meteorology over very rough terrain. The southern half of the base happens to be the most complex, and that is where the launch facilities are located. The northern half of the base is less complex. That is the reason why there are two equations used at Vandenberg.

For cold spills, we also use an Air Force-modified version of the Complex Hazardous Air Release Model (CHARM)™ developed by Radian Corporation. CHARM™ is used specifically for the current program of deactivation of the Titan II missile system. The modified CHARM™ model was added to our pool of models following a thorough investigation of a 1980 hot spill accident of a Titan II near Damascus, AR. As a part of this investigation, a thorough review of the safety procedures for the entire Titan II program was made. One of the recommendations from that review was the need to replace the OB/DG equation. OB/DG does not handle dense gases, such as N_2O_4. CHARM™

does include a dense gas algorithm and has been shown to be useful in the field for estimating a toxic corridor that would result from a release of N_2O_4.

The OB/DG equation is fairly simple. It is based on a linear regression of the data gathered during a large series of test releases. As a meteorologist, it is a little disturbing that the equation does not consider wind speed. This basic equation is even further simplified for the typical Air Force base by adjusting the coefficients and exponents accordingly. We adapted CHARM^{TM} for Air Force use specifically for the Titan II deactivation. It is a Gaussian puff model that includes a dense gas algorithm based on Eidsnik's work. It has a source strength module, while OB/DG does not. Thus, CHARM^{TM} gives us an improved capability in estimating the source strength resulting from a spill.

At the time of a cold spill, by regulation, the Air Weather Service meteorologist on site calculates a toxic corridor. In practice, the response varies. The on-site commander who responds to the spill decides whether the corridor is calculated. This does not mean that no action is taken to prevent loss of life or injury if the modeling is not conducted. Typically, what happens, in my experience, is that the commander responding to the spill directs that the entire downwind area be evacuated. This is a very conservative, but effective approach.

Just as a point of interest, there are several weather restrictions on handling materials, and, frankly, one is a point of contention with some of the maintenance personnel. This limitation was particularly troublesome during the Titan II deactivation that involved quite a bit of transfer of propellants. Essentially, there could be no transfer of propellants during calm winds and/or stable conditions, the stable conditions being determined by the vertical temperature profile. This limitation created a lot of arguments between meteorological and maintenance staffs.

The Air Force has identified several research needs. We need, like most others in this field, improved source strength models. We need a better means of estimating the surface temperature in our models. We are concerned about mixtures of chemicals released to the environment mixing with other chemicals: water, other pollutants, and naturally occurring materials. We do not really have a good model to handle fires, particularly with solid propellants.

We are looking for an improved dispersion model for general use and are still looking for a better replacement for OB/DG, which will consider dense gas effects and incorporate a terrain wind flow model, particularly at Vandenberg. Finally, we need better model validation techniques. The commander on site needs to have some reliable means of quantifying the uncertainty associated with the toxic corridor that is given to him. Frankly, right now we do not have a good means of doing that.

We have several activities under way to meet these research needs. The Air Force Geophysics Lab is working on a new dispersion model. It will be a relatively simple, Gaussian puff model based on the Shell spills model, although we are making several modifications. Most of this effort involves looking at the source strengths involved with spills of the various chemicals about which the Air Force is routinely concerned. We are planning to include a dense gas algorithm. We are also looking at various other models, including the DEGADIS model that was discussed earlier in this conference. A wind flow model, based on work done by the Army, is also being evaluated.

Also, we have initiated a study at Lawrence Livermore National Laboratory to recommend a methodology that could be used by the Air Force when we are faced with the need to do an evaluation of whatever model we finally select. This validation technique will involve compiling the dense gas data that are available in a form suitable for model evaluation and, then, recommending certain techniques to use in comparing our model calculations to the actual field data. We also have a small effort under way to look at quantifying the uncertainty associated with toxic corridor calculations. Additional hot spill models are being considered to fill the current gaps in our capability in that area.

This discussion presents a brief overview of the current capabilities of the Air Force and of the research we have under way to improve our emergency response modeling support capabilities.

POISONOUS GASES FROM LAKES: THE CAMEROON DISASTER

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In 1960, I became interested in poisonous gases because of an experience while on vacation with my family in the crater lake district of Ruwenzori Park in western Uganda. We smelled rotten eggs and tracked the smell about five miles overland with a Landrover, ending up at a small lake that was purple with sulfur bacteria. There was a whitish deposit of salts around the shore. Upwind, the stench was not too bad. We stood there and saw no dead elephants along the edge of the lake, but then, elephants are not usually attracted to drinking water that is supersaturated with halite or trona. It seemed to us the better part of valor not to venture down into the crater to look for smaller dead animals. Elephants might steer clear; limnologists might not.

This incident stayed in the back of my mind for 10 years. When one of my students, John Melack, went to the same lake in 1971, it no longer stank of rotten eggs. The climate of Uganda had changed, with a number of wet years occurring in succession. When Melack got to the lake, it was saturated with respect to sodium chloride in the deep water, but there was a meter and a half of rainwater lying on the surface. There was no evident evolution of gas. On our first visit, we had not observed any bubbles either, but we were probably too far away to see any but catastrophically large ones.

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I have since spent several months on Lake Bosumtwi in Ghana, a meteoritic explosion crater, where there are many traditional reports of large bubbles of gas coming up out of the water. There are even a few reports in the scientific literature of such degassing. Although few people have been killed by these bubbles of gas, accidents have happened with sufficient frequency to generate an interesting folklore regarding the lake and the proper way to propitiate its dangerous resident deity.

The bubbles of gas tend to rise in August. I was there in August, 1966, when the lake was circulating freely. There was no smell of rotten eggs, but the lake had an odor to suggest that some form of reduced sulfur, perhaps mercaptan, was percolating slowly from it. We saw no bubbles of gas burst from the lake.

Last year, Kling and I went to Cameroon with Curt Stager, Jean Maley, and support from National Science Foundation (NSF), Centre National de la Recherche Scientifique (CNRS), and Office de la Recherche Scientifique et Technique d'Outre-Mer (ORSTOM) to study the history of Cameroonian lakes and make a limnological survey of them. Ndoni Paul was our Cameroonian assistant. We arrived shortly after a very big bubble of gas had burst from Monoun, killing 37 people. That happened on August 15, 1984, at approximately 11:30 p.m. On August 21, 1986, at 9:30 p.m., a bubble of gas came out of Lake Nyos in the western part of Cameroon killing almost 1700 people and a great number of cattle. This was a major disaster, comparable to Bhopal and Chernobyl.

When the first reports of a gas discharge came from Lakes Monoun and Nyos, it was regarded as a mystery. Various explanations, natural, artificial, and supernatural, were advanced to explain the mystery. Most of these explanations were less satisfactory to us than they were to others. Now, after the post-event observations of Kling and the other members of the Agency for International Development (AID)-supported Foreign Disaster Team, there is little mystery left. We think we understand the phenomenon quite well. We can probably predict it in a broad sense, and we can almost certainly control it.

These natural events differ from most catastrophes we have been discussing at this workshop. Meteorological processes dissipate this problem, but meteorological processes probably also trigger the catastrophe. They must also be considered in preventing its recurrence.

In a tropical lake, there can be many layers. This layering can be very stable. The first layer is the air-water interface. Next, there is a layer of surface water, usually fairly low in dissolved salts, that circulates freely during the season of minimal thermal stratification in the lake. Underneath that layer, there are usually one or more layers that are stabilized by dissolved substances. These deep layers are not stabilized thermally, and may even display reverse thermal stratification, but are chemically so stabilized that they may be perennial. During the season when the surface water is at its coolest, when the thermal stratification is weakest, a strong wind, low-pressure system, landslide, subterranean slump, or anything else that will disturb the free water surface produces standing waves at all the deep discontinuities.

In a small lake, such as Singletary Lake in North Carolina, the surface rises in the downwind direction on even a fairly still day by something like 5 centimeters. The lakes in Cameroon are also small, with a similar surface setup; but deep in a stratified crater lake, the next discontinuity is set up much more than 5 centimeters in the opposite direction. These two slopes, that of the air-water interface and that of the first water-water boundary, are not the same. The surface slope involves air with a density close to zero and water with density close to one, while the internal slope involves two layers of water with density differences about 1 percent of the density difference at the surface. So, when a wind sets up a lake, the internal slope is some hundred times that of the air-water interface. The vertical displacement will be 5 meters or more.

If a deep layer of the lake, for whatever reason, is charged with a very soluble gas, Carbon dioxide (CO_2), hydrogen sulfide (H_2S), methane, or ammonia to the point of saturation at the ambient pressure, and the layer is displaced by a large set up, then the deep water can effervesce violently. When this happens, we can have a tragedy like that in Nyos or Monoun.

Kling has detailed stratification data from Barombi Mbo, a lake near Kumba in southwestern Cameroon, which fortunately does not have much gas dissolved in its deep waters. Because of the annual pattern of cloudiness, southwest Cameroonian air temperature reaches its annual minimum in August. The surface water of Barombi Mbo also reaches its annual minimum around August. This kind of thermal regime is typical of a tropical lake, which typically has a season of maximum thermal stability with warm surface waters. Stratification involves a temperature range where water density changes quickly with temperature, so small temperature differences are sufficient to produce stable stratification. The upper part of the lake is thermally stable during most of the year, and the deep waters are perennially stabilized by dissolved salts even to the point of allowing a thermal inversion. In June, July, and August, the shallow stability is largely removed by cooling of the surface water. The surface layer and the next layer develop very similar densities. When something sets up the air-water interface, the discontinuity between the surface and deep waters will be set up enough to generate large-scale effervescence of dissolved gas if the deep waters are close to saturation at the ambient pressure. That was apparently the situation at Lake Nyos when it killed 1700 people.

The discharge of gas at Lake Nyos occurred near an 80-meter-high promontory. The initial wave rose over the top of the promontory, and stripped the shallow layer of soil and vegetation from its granitic rocks. That initial displacement generated a surface seiche. The amplitude of the surface seiche was about 6 meters at the far end of the lake. This is obviously a very serious kind of event. It takes a great deal of force to move such an amount of even fizzing water to so great a height.

Maps of the area are poor, and the distribution of dead animals and people have not been plotted with a high level of accuracy. The village of Old Nyos, which is 100 meters or more above the lake was not affected. Observers in Old Nyos, who were awake at 9:30 p.m., claim to have seen the burst of gas and water from the lake, but no one died there. On the other side of the lake at Sawe, which is not so high above the lake, no deaths occurred either. However, downstream from the lake the village of New Nyos was wiped out. The fairly heavy settlements along the road following the river, as far as Su Bum, were also wiped out. At that point, the river takes a turn and passes through an area that is lightly inhabited, until it reaches the village of Mashi, where again there were very heavy deaths. The distance along the course of the river from Lake Nyos to Mashi is about 34 kilometers. The width of the valley is not well known, but from the map contours we estimated it to be about 2 kilometers wide. If the valley were 2 kilometers wide and if it were filled with gas to a depth of 10 meters, then we are talking about something like 7×10^8 cubic meters of gas.

Autopsy reports indicated that the people died of CO_2 poisoning. There was no indication of carbon monoxide (CO) or hydrogen cyanide (HCN), nor was there any indication of H_2S in the victims. They died of CO_2 poisoning.

If the lake, which is very deep for its size (1 kilometer by 2 kilometers, with a maximum depth of 220 meters), were fully charged with CO_2, it would hold about 10^{10} cubic meters of CO_2. This is sufficient to fill the valley more than 10 times. An amount of gas that would fill the valley, if expanded from 22 atmospheres to atmospheric pressure, could do a lot of work. It could easily lift a destructive wave of water to a height of 80 meters. Remember, the entire volume of the lake is not being lifted, but only a small portion of one side. It struck the promontory with enough force to splash over the top, even though the water surface generally was not raised that high.

What was the source of the gas? The limnologist thinks first of detritus, the corpses and feces of lake-dwelling plants and animals that decompose as they settle to the bottom. This decomposing material generates CO_2 by aerobic respiration and by fermentation together with methane when the oxygen is depleted. Ammonia and H_2S are also generated under anoxic conditions. It turns out that the CO_2 in the lake cannot come solely from biological processes. There is proportionately too much CO_2 and not enough of the other products of decomposition in the gases of Nyos and Monoun. There is not enough methane, H_2S, or ammonia. If the gases in the deep waters of the lake contained appropriate amounts of biologically derived ammonia, water samples from the lake would bring tears to your eyes. While there is ammonia in Lake Nyos waters, there is not enough to support a theory of biological origin for the CO_2.

The isotopic ratios of gases in the lake waters also provide clues. The first U.S. team to sample Lake Monoun last year found that the CO_2 in the water had a radiocarbon age of 18,000 years. This suggests that perhaps one-eighth of the CO_2 came from biological processes. The remaining seven-eighths came from some other, non-biological source. These ratios are consistent with various mixtures of primeval CO_2, i.e., CO_2 coming from magma. Overall, the evidence indicates that approximately one-tenth of the CO_2 was coming from a biological source, and the remaining nine-tenths, probably, from deep springs. Looking at Cameroon's springs, we find that most, particularly those of West Cameroon, are effervescent and that most are a good source of CO_2.

In each of the papers we have heard at this conference, we learned about opportunities to select sites, to design plants, or to develop emergency response plans as an effective means of dealing with environmental emergencies. Such plans are not helpful in Cameroon. If you are ever caught in a Cameroonian CO_2-release emergency, the only thing you can do is hold your breath and run uphill. You are very much better off suffocating from lack of air than breathing dense concentrations of CO_2. Breathing the CO_2 causes severe acidosis, your brain shuts down in seconds, your glottis goes into spasm, and you die quickly.

What can you do in a situation where you cannot select your site by moving away and raising your crops elsewhere? You may be able to modify the site. It is possible to take a pipe, of perhaps 6 inches in diameter, put it down into the deep water of a lake that is fully charged with CO_2, and pump the water up with a pump until it effervesces. Then, you can shut off the pump and sit back and watch the lake degas. It would take about 10 years by this method to discharge a lake the size of Nyos to saturation at surface pressure. But do not forget meteorology while degassing the lake. First, you must know where your discharge plume will travel. Second, you must take care how fast the lake will degas: too fast, and you might produce your own small catastrophe; too slowly, and the springs can keep up with you, and you will never get rid of the CO_2. There also must be a limnological portion to your plan. When the pipe is running, you must dispose of the waste water carefully. If it is returned to the lake in a turbulent fashion and mixes freely with the upper layer of the lake, you may generate a catastrophe worse than any happening naturally.

SUMMARY OF PANEL DISCUSSIONS

Panel discussions were organized to directly address the goals of the workshop and to provide a forum for free discussion of the issues raised by the goals. The panelists and participating workshop attenders sometimes followed an independent agenda, but the resulting discussions were very fruitful.

Panel 1: Summary of Current Status of Source Strength and Dispersion Models, Their Strengths and Weaknesses, and Recommendations for Improvement

Panel 2: Recommendations for Selection from Among Current Models for Immediate Use in Hazard Identification and Evaluation, Preparation of Emergency Preparedness Scenarios, and in Response to Emergencies

Panel 3: The Role of the Meteorologist in Hazard Evaluation and Emergency Response

One major accomplishment of these panel discussions was the fostering of strong interactions between two technical communities present at the workshop. The people involved with chemical releases seldom have interacted directly with those involved in radioactive releases. The difference in viewpoint was profound. For example, Dr. Knox related his experience with Chernobyl and showed how the source term could be inferred from measurement of the radioactive debris. This procedure took several days, but as his major concern was the impact upon the United States, this time interval was not important. Even if the concern was for European exposure, there was time to take measurements and estimate the source term. On the other hand, Dr. Galt showed that when one is dealing with an overturned vehicle, immediate

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estimates of the source term and the relevant species are required immediately, especially if evacuation of people is contemplated. Between these two extremes was a continuous spectrum of concerns. The panels allowed for a free expression of these concerns and thus proved useful.

Panel 1: Summary of Current Status of Source Strength and Dispersion Models, Their Strengths and Weaknesses, and Recommendations for Improvement

Chairperson: Frank Schiermeier
Reporter: Steve Perry

Panel Members: Gary Briggs, Tony Cox, Don Ermak, Dan McNaughton, Bob Meroney, Jerry Schroy

This panel summarized the current status of source strength and dispersion models, especially their strengths and weaknesses, and recommended necessary improvements. Four major areas were addressed: source term models, dispersion models, evaluation and validation of models, and practical application of models.

Knowing how much material is emitted in a given emergency situation is of primary importance. Most often the emission rate is estimated by means of a model calculation. The panel reported on five source term model categories: process emissions, contained emergency releases, spills, burning sources, and density impacts. Process emissions are usually point sources from established stacks and are thus well documented. Contained emergency releases result from components designed to release material under certain conditions. Examples of these are discharges from relief valves and rupture disks.

The material released could be from a runaway reaction, which requires careful engineering judgment. If the material is accidentally or deliberately ignited, there would be a burning source, which is discussed further below. Finally, if the material is stored under high pressure, the release would be a jet that might produce a multiphased flow. This last case is not well understood at all and requires a great deal of careful research. Spills of pure components and binary mixtures that undergo simple flashing and pool formation are reasonably well understood. Spills that involve multiphase flows are, again, not well understood. Steady-state spill models are useful for situations that are most nearly steady (obviously). As the conditions depart from steady-state conditions, such as occurs with pressure drops, the steady-state models decrease in usefulness. There is a very strong coupling between source models and dispersion models for spills that involve aerosols and evaporation from these aerosols. In fact, it is virtually impossible to separate the two for some conditions.

Burning sources are another category where there are major unknowns and much research to be done. A relatively simple burning source would be a flare that resulted from igniting a contained emergency release. The input products are known; so presumably would be the combustion products. This is not always true because combustion may be strongly influenced by the ambient meteorology and any mitigation techniques that might alter the combustion temperature. The reaction products often are controlled by the combustion temperature. Thus, even a flare is not well enough understood. With an open burning source, the unknowns multiply very quickly. The combustion temperature is unknown, the product species are unknown, and the effect on material that is not burning but adjacent to the fire is unknown. Furthermore, attempts to extinguish the fire may make the situation worse by making the species emitted more toxic than the original combustion products. Major research is needed here.

The density impact source category is a general category for which parameters like aerosol formation from condensation, partial vaporization, chemical reaction, initial dilution, and source temperature are important. The single most important point about density impact sources is the very strong nonlinear effect between the size of the source release and the subsequent behavior of the dispersing plume. Here again, there is a very close coupling between the source term and appropriate dispersion model. The panel reported three major dispersion modeling categories related to plume buoyancy: nonbuoyant, positively buoyant, and negatively buoyant plumes. The nonbuoyant or passive plume category applies to all plumes after enough dilution. The character of the planetary boundary layer (PBL) is the most important variable here. If the PBL is unstable, i.e., large convective eddies driven by the surface heat flux dominate the turbulent exchange, the dispersion of passive plumes is quite well understood. The models developed for this case do much better than the Gaussian models. This is rarely a worst case (where very high concentrations occur) since dilution is quite rapid. For the neutral case where the turbulent exchange is dominated by eddies generated by the vertical wind shear, the Pasquill-Gifford type Gaussian model does an adequate job. But, this is only true for the near-ideal cases in smooth flat or gently rolling terrain. This, also, is seldom a worst case, because there is often adequate mixing and dilution.

The passive plume in stable conditions is often the worst case scenario, as well as the most difficult case to model. The Pasquill-Gifford method only works for smooth terrain and unrestricted mixing height (an unlikely occurrence). The passive plume in stable conditions is the hardest case to generalize because of surface roughness effects, limited vertical mixing, flow meander, and drainage flows in sloping terrain with the possibility of channeling. This case requires an extensive research effort.

Buoyant plumes from stacks are reasonably well modeled with current methods. Surface releases are very difficult to model because of surface deposition, high turbulence levels, and entrainment effects. If the plume is buoyant enough, it will lift from the ground. Buoyant plumes interact with the PBL and will reach greater heights during convective conditions and will be restricted in stable conditions, especially if the buoyancy is insufficient to completely penetrate the nocturnal stable layer.

A special type of buoyant plume that has not been well studied is the flare. Often, a mitigation technique for a release is to burn the material in a flare. An example is a release of hydrogen sulfide, which would be converted to sulfur dioxide after combustion. The detailed consequences of such an action under all possible PBL conditions are unknown at present.

Dense gas plumes are currently the subject of intense interest because of their potential for immediate health consequences. A dense plume is one that is negatively buoyant under all atmospheric conditions. Such plumes often modify the atmospheric conditions locally that can inhibit dilution. The current view is that in sloping terrain, with slopes as small as 0.1 percent, these plumes will travel downslope. With an adverse wind, this might not be the case, however. In complex terrain, such as canyons with steep walls, a dense gas can travel great distances as the event in Cameroon showed. Much work needs to be done to characterize dense plume behavior in complex terrain, especially with different wind fields. In terms of accidents, however, the most important questions concern the direction a dense gas cloud will travel in real terrain with real wind speeds and directions, and what the concentration field will look like.

One technique that should be explored for all possible source and dispersion situations is the use of virtual sources that can be nondimensionalized. One mathematical model then could be used for a variety of releases. Some problems, of course, cannot be treated in this manner because of their inherent nonlinearity, e.g., a burning source.

Dispersion models cannot deal satisfactorily with complex terrain and winds of very low speed to calm, nor can they deal with the transition from near source density-dominated dispersion to far-field passive dispersion. There has been little effort to include spatial and temporal variability into current dispersion models.

Introduction of new or improved models into the inventory of operational models requires a demonstration that the new models are indeed improvements. For cases where there is no current model, a rigorous comparison of model results with data is most important. For cases where there are current models, the new models must show a clear improvement. Further, all new models should undergo extensive sensitivity testing. In addition to the sensitivity analyses, a set of cases where previous models have failed should be developed and the new model tested on these cases to ensure correct model performance.

The panel concluded that in selecting a suitable model for application, several issues must be considered. In hazard identification, the emphasis is on source characteristics, i.e., the possible ways in which the source could emit hazardous material. The models required for this phase of emergency response concern the different types of accidental spills that can occur along with a good engineering estimate of the probability of such an accident. Emergency action planning requires the results of the hazard identification study followed by consideration of all possible ways in which the release can be influenced by weather conditions. The models required must account for the transport and dilution of the released effluent. Chemical transformation of some species must also be considered.

A family of concentration isopleths for a variety of release scenarios and environmental conditions are developed. This information can be viewed together with appropriate demographic data to estimate human exposures to the hypothetical releases. This last step should result in a plan for responding to accidental releases. Emergency response requires immediate answers for alleviating the risk to the public. The models used must be able to be run on very short notice with unambiguous results. If hazard identification and preparedness planning processes are done correctly, then there should be a menu of recommended actions from which to choose. If enough cases were examined in the planning stage, then there should be a close analogy to the actual accident. Appropriate action can then be taken.

Panel 2: Recommendations for Selection from Among Current Models for Immediate Use in Hazard Identification and Evaluation, Preparation of Emergency Preparedness Scenarios, and in Response to Emergencies

Chairperson: Ray Hosker
Reporter: Tom Pierce

Panel Members: Harry Allen, Jerry Galt, Jerry Havens, Reed Hodgin, Gene Runkle, Bruce Turner

The second panel considered recommendations for selection of models for immediate use in hazard identification and evaluation, preparation of emergency preparedness scenarios, and for response to actual emergencies. The panel did not recommend specific models, but rather agreed to a list of features and technical criteria for model choice.

The first general feature was scientific defensibility. The scientific basis of a model for a particular application is of great importance. The model should be operated only for those situations where scientific credibility has been established. The model should be widely available with full documentation on both the scientific basis and on test results showing how the model performs over the full range of applicability. The documentation should also include all technical criticism and responses to this criticism. Further, the model structure should be organized into modules that allow updates to be easily installed. Each model should have been subjected to rigorous peer review and all results of the review available to the user community.

The panel recommended a number of technical points that models should deal with:

1. Near calm to very light winds
2. Wind shear in the vertical (speed and direction)
3. All stability conditions
4. Site-specific meteorological data
5. Local terrain and local flow conditions
6. Local obstructions
7. Dense gas effects
8. Effects of hydrometeors (rain, snow, etc.)
9. Momentum and buoyancy effects at the source
10. Time-varying release rate
11. Chemical reaction of effluent
12. Real time on-site concentration measurements.

As is obvious from this list, the panel determined that the problem of application of models was very much dependent upon the individual case and that no global recommendation of a specific model for all cases was possible. Rather, a suite of models, each carefully matched to the others in the suite, was the best approach.

The panel next recommended that potential model users examine the suitability of a given model with the following guidelines. First, for application to toxic releases, the effects of the toxicity and a probabilistic statement of associated risk should be incorporated into the model output so that the user is able to relate this output to the problem at hand without going through another step. Second, the model should be capable of producing results commensurate with the level of accuracy actually required in the application.

The panel considered the issue of possible categories for model use. The first use is for hazard identification. Does a given situation pose a hazard to the public? The best approach here is to do an analysis of possible release scenarios, then use the model most applicable for that case. Since rapid turnaround of results are not necessary for this situation and realistic estimates are desired, the model should be as complete a representation of the situation as is scientifically possible. The second possible use identified was preplanning for the possible occurrence of the releases that posed hazards. As before, the model should be as complete and realistic as possible. Response plans should be developed using these results. The third model use category occurs when and if an actual release occurs; a simple model with quick turnaround is most appropriate. Of course, this quick turnaround model should have been run in the planning stage so that a record of its performance relative to the most complete model is available. Thus, a check on the uncertainty of the simple model's results are available to the user, and safety factors are incorporated into response plans that are to be activated. The final model use category is for post-event analysis. The most complete model should be used along with simple model results to assess the performance of the entire emergency response system.

The panel recommends that all emergency response plans be thoroughly tested. These plans can be tested by holding simulation exercises to ensure familiarity with all components.

Panel 3: The Role of the Meteorologist in Hazard Evaluation Emergency Response

Chairperson: Lew Nagler
Reporter: Jack Shannon

Panel Members: Marvin Dickerson, Allen Weber

The role of the meteorologist in hazard identification, emergency preparedness planning, and in emergency response is multifaceted but must remain closely connected with his or her expertise. This expertise should include some knowledge of allied fields such as industrial hygiene and health physics because the advice sought most often is related to these fields.

In hazard identification, the role of the meteorologist is to advise on how a given potential hazard might be affected by weather conditions. For example, in analyzing the risk for a release from some storage or processing facility, the wind field and atmospheric stability determine the rate of dilution for the released material. The details of the source configuration as well as any proposed mitigation techniques are very likely affected by meteorological conditions. Thus, a meteorologist should be consulted at the very start of a hazard identification exercise.

In terms of emergency preparedness, the meteorologist will select the appropriate models for the problem and will be able to advise on the most probable exposures arising from a given release. He or she will also select the models to be used in the event of a real emergency and demonstrate how the operational model handles the same situations simulated by the more sophisticated planning models. Finally, the meteorologist will prepare weather scenarios for initial training in emergency response and will also provide real data for further training exercises. The meteorologist will also advise on the most appropriate placement of on-site instrumentation (both weather sensors and chemical or radiological).

For actual emergency response situations, the meteorologist will have to provide the weather data and model predictions for use by the appropriate authorities. If the meteorologist has been included in this process from the beginning, then this last phase, which is the most difficult, will be that much more reliably done.

APPENDIX A

The Bhopal Gas Tragedy

THE BHOPAL GAS TRAGEDY

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Abstract

In the early hours of December 3, 1984, about 40 tons of highly toxic, volatile, and reactive methyl isocyanate (MIC) and other poisonous gases leaked from a storage tank at a pesticide plant in Bhopal, India. The gases escaped in about 90 min through a 33 m high atmospheric vent into the cool night air, and quickly spread in a foglike lethal cloud over a large populated area. Thus began the world's worst industrial disaster involving toxic chemicals which killed over 2,200 people and injured more than 200,000.

In this paper, we sketch the accident scenario and outline the events in the aftermath of this catastrophe. The topographical features and meteorology of Bhopal, and the physical, chemical, and toxicological properties of MIC and other gases in the leak are described in the context of the dispersion of the cloud and its effects on human and biological life. A simple atmospheric dispersion model, emphasizing aqueous phase conversion and deposition of MIC, is presented. This model, based on an analytical solution of the 3-D advection-diffusion equation, gives estimates of ground-level concentrations and deposition fluxes of MIC. The model estimates are qualitatively correlated with recorded human fatalities and injuries, and the observed damage effects on trees and vegetation in the affected areas.

In the epilogue, the medical care, relief and rehabilitation efforts, and some preliminary results of the ongoing medical and toxicological studies are summarized. The legacy of the Bhopal Tragedy including its implications for information, siting and operation of plants that handle toxic chemicals, safety, health, and environmental standards and enforcement, emergency response programs, and other relevant issues, are briefly discussed.

Presented at the Special Joint Session of the Ocean and Atmospheric Sciences on "Paths and Fates of Toxic Pollutants in the Atmosphere and Oceans," American Geophysical Union Fall Meeting, Dec. 7-12, 1986, San Francisco, CA.

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INTRODUCTION

On the night of December 2-3, 1984, at around midnight, methyl isocyanate (MIC) and other poisonous gases, escaping from the Union Carbide India Ltd. (UCIL) pesticide plant in Bhopal, silently spread out into a huge cloud that enveloped a large populated area of the city. Hundreds, mostly children and old people, died in their beds. Thousands more awoke to a Kafkaesque nightmare of suffocation, blindness, and chaos, and stumbled into the streets, joining human stampedes fleeing the gas cloud. In the confusion, some ran in the direction of the wind and died along the way. Many others died later in hospitals. Thousands more were injured due to exposure to the toxic gases. In all, over 2,200 people died, and more than 200,000 were injured. Thus, "Bhopal" came to be associated with the world's worst industrial disaster involving toxic chemicals.

TOPOGRAPHY AND METEOROLOGY

Bhopal was an unlikely setting for this tragedy. A city of about 1 million people, 600 km south of New Delhi, Bhopal (lat. 23°17'N) is the capital of Madhya Pradesh, India's largest state, with an agriculture-based economy. Because of its central location, resources, and hospitality, the state traditionally attracted people from all parts of the country to work in its 8000 industrial plants of various sizes. Bhopal was once a center of India's mogul past, and the city still reflects this history despite a skyline of modern state office buildings, colleges and hospitals built around two ("Upper" and "Lower") lakes.

The UCIL pesticide plant is located in the northern parts of the city (Figure 1). North of this facility, there are hillocks, woods, and stretches of residential areas extending out to 24 km from the plant. The Indian Agricultural Research Insitute is situated about 4 km north of the UCIL factory. The latter is surrounded by residential areas on the other three sides. The approximate distances and locations, with respect to (w.r.t.) UCIL, of some Bhopal landmarks shown in Fig. 1 are as follows: Electrical and Mechanical Engineers (EME) Center (1.5 km W), airport (6 km W), Hamidia Hospital (3 km SW), Sultania Hospital (3 km S), the State Secretariat (Vidhan Sabha) and Police Headquarters (PHQ) (4 km S), and the Railway Station (1.5 km SE). An industrial and warehouse area extends out to 15-20 km on the plains ESE of the plant along the railroad.

Table 1 shows the elevations and locations (w.r.t. UCIL) of some of the important topographical features of Bhopal. Some of these features could have influenced the local wind and dispersion patterns on the night of the accident.

Detailed meteorological data are not available regarding the wind speed and direction, and the vertical temperature structure at the site on the night of the accident. According to Ekalavya (1985), a private non-profit organization based in Bhopal, the winds that night were initially from the northwest and subsequently from the north. Post-episodic wind data indicate that the most probable wind speeds were of the order of 3 m/s. The temperature was reported to be 14°C.

Table 1. Elevations and Locations of Bhopal's Topographical Features.

	Elevation (m) above MSL	Distance (km) & Direction (w.r.t. UCIL)
Singarcholi Hillock	625	4.5 W
Idgah Hill	575	2.0 WSW
Ahmadabad Hill	513	2.5 WSW
Dharampuri Hill	601	5.5 SW
Birla Temple Hillock	562	4.5 SSE
Shahpur Hill	525	8.0 SE
Upper Lake	-	4.0 SW
Lower Lake	-	4.0 S

This is consistent with the minimum winter temperature of about 10°C in Delhi. Since both cities are located in the Indo-Gangetic plains, a mixing height (H) of 200 m, close to its climatological-mean value in Delhi (Kumari, 1985) for a December night, was assumed for Bhopal.

The gas-affected areas in Bhopal are characterized by a gently rolling terrain surrounded by hillocks and lakes. It was likely that nocturnal drainage winds and land breezes altered the local surface wind patterns on the night of the gas leak. In the absence of data, the best way to decide on the wind direction is by charting the course of the catastrophic imprint of the poisonous gases over the city. Interviews with survivors and rescue personnel confirmed that the wind direction varied during the night. Based on this information, Singh and Ghosh (1985) adopted the following sequence of wind directions, apportioned appropriately for the duration of the episode: (i) 285° for 45 min, (ii) 340° for 30 min, and (iii) 45° for 15 min. This scheme gave realistic model simulation results, as described later.

THE ACCIDENT AND ITS AFTERMATH

The UCIL factory in Bhopal employed 950 people to manufacture and market Sevin (carbaryl) and Temik (aldicarb), two MIC-based pesticides. The accident began on the night of Sunday, December 2, 1984, when about 75 workers were on duty. As reported in the biweekly India Today, which investigated the accident and reconstructed it with approximate timings, the sequence of events (in local time) is as follows:

10:45 pm - A shift change occurred at the factory. Unknown to the incoming shift, a runaway chemical reaction was already under way in storage tank 610, which contained 41 metric tons of liquid MIC.

11:00 pm - Pressure in tank 610 was observed to increase from 3 to 10 psi. The new staff mistakenly thought this was due to nitrogen pressurization of the tank by the previous shift.

11:30 pm - Operating staff noted eye irritation but ignored it, because tiny leaks of MIC in the utility area were not unusual.

00:15 am - MIC control room staff reported the high pressure (30 psi) in tank 610 to the Production Assistant; he checked and found that the tank's rupture disk (designed to rupture at 40 psi) had burst, and the safety valve had popped.

01:00 am - Untreated MIC vapor was seen escaping through the 33 m high atmospheric vent line. Within a period of 90 min, about 40 tons of MIC leaked out in gaseous form.

The escaping gases overwhelmed the scrubber designed to detoxify process vent gases. Other elaborate safety systems that failed included the flare tower, the refrigeration system, and the water curtain (which was designed to shoot water to a height of only 15 m), and some of the other systems which had been out of operation for repairs. The public warning siren was turned on for a few minutes around 1:00 am, but was not sounded again until 2:00 am. The city police control room was alerted, just after 1:00 am, by a town inspector on patrol near the factory. The police, in turn, alerted the area hospitals, the army, and the state medical director at 1:30 am.

The poisonous gases emerging from the vent stack formed a huge white cloud that moved south towards the densely populated areas. In the vicinity of the plant, according to survivors' reports, the gas was so thick that visibility was very low. More than 200 people died in their beds in the area immediately south of the plant. Others awoke to a feeling of suffocation and burning eyes, and rushed out of their homes in panic. In the narrow streets, they joined tens of thousands of half-blinded people running for their lives. It must have been a terrifying spectacle. Hundreds were overcome as they fled. Many collapsed on the roads, only to be removed to the hospitals later. The cloud engulfed Bhopal's railway station as it spread southeast from the plant. Passengers and station personnel collapsed. As humans died, so did animals. The carcasses of dogs, cats, chickens, birds, goats, cows, and other animals were later found strewn over an area of 65 km^2 in the quadrant SE of the plant.

Starting about 2:00 am, the first victims began arriving at Bhopal's hospitals. Buses, army trucks, ambulances, and private vehicles were pressed into service. All seven of the city's hospitals were beseiged by thousands of gas victims. Doctors, joined by interns, nurses, and medical students, began a seemingly unending battle to save lives. As the hospitals became jammed, doctors, relief agencies, and private groups set up emergency clinics on sidewalks, in stores, and wherever they could find space. Bhopal's medical community rose to the occasion to handle the emergency resulting from the unprecedented disaster and performed heroically in saving many lives.

A house-to-house search of the affected areas turned up hundreds of victims. By late afternoon, the city morgue was overflowing with bodies, many of them unidentified. There were mass burials and cremations for the dead. As dusk fell the death toll mounted to over 1000 and the number of injured rose to more than 100,000. As the magnitude of the tragedy became apparent, additional medical personnel, equipment, and relief supplies were rushed to the city.

CHEMISTRY AND TOXICOLOGY

Methyl isocyanate ($CH_3N{=}C{=}O$) is a reactive, toxic, volatile and flammable compound which is commercially used to make carbamate pesticides. MIC, an ester of isocyanic acid, is industrially produced by the reaction of phosgene ($COCl_2$) with the base methylamine (CH_3NH_2):

$$COCl_2 + CH_3NH_2 \longrightarrow CH_3N{=}C{=}O + 2\,HCl \qquad (1)$$

It should be noted that MIC is stored with a purity of 99.5%, and contains up to 0.1% phosgene to inhibit MIC polymerizations and reaction with water. Thus, 40 tons of MIC (in tank 610) could also have contained up to 40 kg of phosgene.

MIC undergoes exothermic and vigorous reactions with a variety of compounds containing active hydrogen atoms. The cumulative effect of the adjacent double bonds adds to the instability of the compound. From a practical point of view, only a limited number of those reactions could conceivably have taken place in the plant at Bhopal (depending on the presence of specific reactants during the episode). These possible reactions are shown in Table 2. Post-episodic analysis of sludge samples from tank 610 showed that two major reactions took place in the tank -- that of MIC reacting with water, and that of MIC reacting with itself, catalyzed by iron, which is a much faster reaction. More than 50% of the sludge was found to consist of MIC trimer resulting from the latter reaction, which liberates about 1.26×10^6 joules of heat per kg of MIC. About 16 to 28% of the sludge was made up of compounds produced by MIC reacting with water, which starts off slowly at room temperature, producing about 1.36×10^6 joules of heat per kg of MIC. Just a small amount of water with a trace of contaminants such as rust and salt, for example, could catalyze an autoreaction. The heat liberated during an induction period lasting a few hours could generate a reaction of explosive violence. It is not hard to imagine situations in which such trace contamination could occur, despite best efforts at prevention.

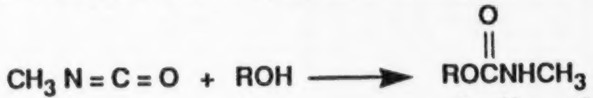
Though the initial mix of poisonous gases that escaped from the factory into Bhopal's air primarily consisted of MIC, it apparently also included smaller amounts of phosgene, hydrogen cyanide, methylamine, and other gases such as carbon monoxide. Though officials initially denied any possibility of cyanide presence, scientists detected cyanide near the MIC storage tank, and 50 m downwind, three days after the accident. Further, autopsies confirmed symptoms of cyanide poisoning among some of the victims. During the runaway reaction in tank 610, it is possible that temperatures exceeding 200°C were attained. At these high temperatures, MIC can break down into hydrogen cyanide, carbon monoxide, mono-methylamine, and some organic cyanides. The physico-chemical, and toxicological properties of various poisonous gases in the Bhopal tragedy are given in Table 3.

The behavior and fate of a MIC plume in the environment is schematically shown in Figure 2. In the atmosphere, MIC reacts with moisture to yield methylamine (MA) and CO_2:

$$CH_3N{=}C{=}O + H_2O \longrightarrow CH_3NH_2 + CO_2 \qquad (2)$$

Table 2. Some Important Chemical Reactions of MIC.

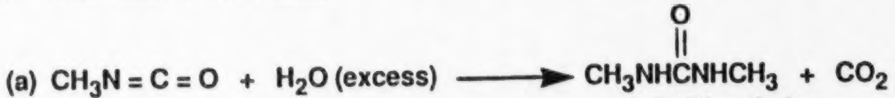
1. Reaction with alcohols and phenols



$$CH_3N=C=O + ROH \longrightarrow RO\overset{\overset{O}{\|}}{C}NHCH_3$$

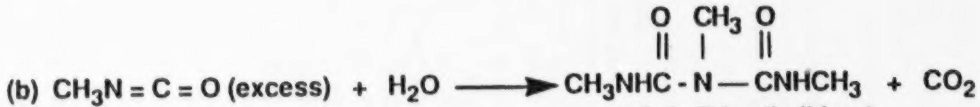
An N-methylcarbamate

2. Reaction with water



$$\text{(a)}\ CH_3N=C=O + H_2O\text{ (excess)} \longrightarrow CH_3NH\overset{\overset{O}{\|}}{C}NHCH_3 + CO_2$$

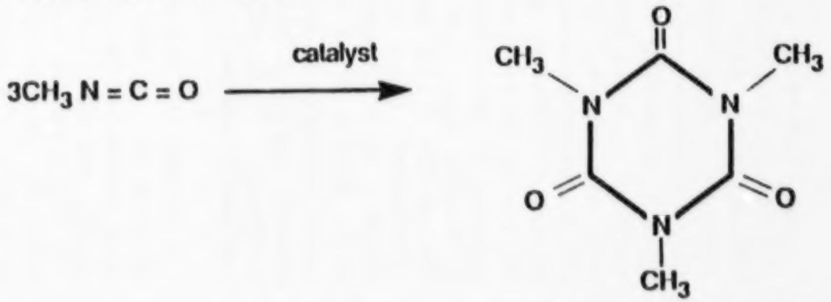
1, 3 - Dimethylurea



$$\text{(b)}\ CH_3N=C=O\text{ (excess)} + H_2O \longrightarrow CH_3NH\overset{\overset{O}{\|}}{C}-\overset{\overset{CH_3}{|}}{N}-\overset{\overset{O}{\|}}{C}NHCH_3 + CO_2$$

1, 3, 5 - Trimethylbiuret

3. Reaction with itself



Trimethyl isocyanurate

Table 3. Physico-Chemical and Toxicological Properties of MIC and Other Poisonous Gases in the Bhopal Tragedy.

	MIC	Phosgene	Hydrogen Cyanide	Methylamine
Chemical formula	$CH_3N{=}C{=}O$	$COCl_2$	HCN	CH_3NH_2
Description	colorless liquid with powerful odor	colorless gas or volatile liquid	colorless liquid with faint odor of bitter almonds	colorless liquid or gas with strong odor of ammonia
Mol. Weight	57.05	98.92	27.04	31.06
Boiling Point (°C)	39.1	7.6	25.7	-6.3
Liquid Density (w.r.t. water) (@ 20°/4°C)	0.96	1.38	0.69	0.66
Vapor Pressure (mm of Hg)	348 (@ 20°C)	1180 (@ 20°C)	400 (@ 9.8°C)	-
Vapor Density (w.r.t. air)	2.2	3.4	0.93	1.07
LC_{50} (ppm) (rats)	5 (4 hr)	1482 (1 min)	544 (5 min)	-
LC_{50} (humans)	>20* ppm	3200 mg/m^3	200** mg/m^3	-
TLV-TWA (ppm)	0.02	0.1	10	10

References: Sax (1979), Weast (1982).

LC_{50}: The concentration lethal to 50% of a specified population.

TLV-TWA: Threshold Limit Value-Time Weighted Average. (The average concentration for an 8-hour workday to which workers may be repeatedly exposed without adverse effect).

* Estimated as 1000 times TLV-TWA value.

** Lowest published lethal concentration for a 10 min inhalation.

Similarly, phosgene reacts with moisture to yield hydrogen chloride and CO_2. In the presence of sunlight, MIC degrades into polymers and gases such as CO and N_2. In soil and water, methylamine is the major product. It is held tenaciously by soil particles until decomposition is accomplished by weathering and biological reactions. In plants, MIC could have competed with CO_2 in the process of photosynthesis. It could have been transformed into methylamine and other carbamylated derivatives of the plant constituents.

One of the disturbing aspects of the chemical disaster at Bhopal is that scientists know relatively little about the toxic effects, especially the long term ones, of MIC. Good toxicological data on MIC were non-existent in the open literature. The permissible MIC skin exposure limit is 0.02 ppm averaged over 8 hrs. This threshold limit value (TLV) has been set by the American Conference of Governmental Industrial Hygienists (ACGIH). It represents the time weighted average concentration (for a normal 8 hour day or 40 hour work week) to which nearly all workers may be repeatedly exposed, day after day, without adverse effect. Isocyanates long have been known to attack the respiratory system, eyes, and skin. They can injure the lungs and bronchial airways, and cause permanent eye damage. But until the Bhopal episode, the effects of MIC had never been observed on such a large and diverse population. Most of the deaths have been attributed to various forms of respiratory distress.

Indian scientists have initiated a variety of studies to investigate the long-term consequences of exposure to MIC. Many of these research efforts are focused on damage to specific organs, such as the eye or lung. Others address possible genetic and carcinogenic effects. The value of all these clinical and laboratory studies, which may take up to 3 to 5 years, will largely depend on building a data base of high-quality epidemiological information. For this purpose, researchers need to answer at least three key inter-connected questions:
(i) Where were the victims when they were exposed to the gas?
(ii) What dose did the victims encounter?
(iii) What were the health effects from exposure to the gas?
The most difficult part of this investigation will be to estimate the concentrations of MIC that individuals encountered. One indirect way to estimate the MIC concentrations is by charting the degree of damage to sensitive trees and plants in different parts of the city; this will enable one to determine the level of MIC to which people in those areas were exposed. Scientists from the Indian Agricultural Research Institute and the Central Board for Prevention and Control of Pollution studied the trees and crops in Bhopal immediately after the disaster.

Another indirect way to estimate the concentrations is through the use of a suitably formulated atmospheric dispersion model. Singh and Ghosh (1985, 1987) have developed a simple analytical dispersion model including the aqueous phase transformation and deposition of MIC, as described below, for use in preliminary assessments.

DISPERSION MODEL, RESULTS, AND CORRELATION WITH OBSERVED EFFECTS

The density of MIC vapor is about twice that of air. This suggests that density effects might be important for plume dispersion. However, the velocity of ejection of the gas was very high and, hence, there was probably considerable entrainment and mixing. Exothermicity of the MIC-moisture reaction suggests that a great deal of heat was generated in the process, and this could further reduce the density of the plume. As a first approximation, therefore, the density effects were not explicitly considered in the model. The plume dispersion was assumed to consist of spreading due to passive diffusion as well as spreading due to gravitational effects; this would imply larger σ values than in the case of a purely passive diffusion. Singh and Ghosh (1985) found that Briggs' (1973) urban dispersion parameters for stable conditions (E-F) give concentration estimates that were consistent with the observations. Other assumptions used in their model formulation were as follows: (i) the time-dependent emissions are specified by a uniform emission rate over the duration of the episode, (ii) the terrain is flat and spatially homogeneous, and (iii) removal by dry deposition and chemical transformation is a first-order irreversible process.

The time-dependent three-dimensional atmospheric advection-diffusion equation is given by

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - k_t C \tag{3}$$

where C(x,y,z,t) is the pollutant (MIC) concentration, U is the constant average wind speed along the x-direction, k_t is the total removal rate, and D_y and D_z are the constant eddy diffusivities in the crosswind and vertical directions, respectively. The source condition is described by

$$C(0,y,z,t) = \frac{Q(t)}{U}\,\delta(z-h_s)\,\delta(y) \tag{4}$$

$$\text{where} \quad Q(t) = \begin{cases} Q_0 \, , & 0 < t \leq t_e \\ 0 \, , & t > t_e \end{cases}$$

In Eq. (4), Q_0 is the MIC emission rate, h_s is the effective release height, and $t_e = 5400$ s is the duration of the release. The initial and boundary conditions are given by

$$\begin{aligned} C(x,\, y,\, z,\, 0) &= 0 \\ D_z \left.\frac{\partial C}{\partial z}\right|_{z=0,H} &= 0 \\ C(x\,,\pm\infty,\, z,\, t) &= 0 \end{aligned} \tag{5}$$

The total removal rate (k_t) of MIC is given by

$$k_t = k_c + k_d \tag{6}$$

where k_c is the chemical reaction rate and k_d is the dry deposition rate. Singh and Ghosh (1985, 1987) considered the diffusive mass transport of MIC by aqueous phase reactions in spherical droplets, following the approach of Reid and Sherwood (1958) and Schwartz (1984). Assuming an atmospheric liquid water content of 0.17 cm^3/m^3, they estimated the aqueous phase reaction rate (k_c) of MIC in the atmosphere as

$$k_c = 7.265 \times 10^{-4}\ s^{-1} \tag{7}$$

The dry deposition removal rate is evaluated from $k_d = V_d/h$, where h is the depth of the gas layer, and V_d is the dry deposition velocity. Because of its high reactivity and affinity for water, the atmospheric behavior of MIC gas is characterized by a low residence time of the order of a few hours, similar to that of nitric acid vapor; therefore, the deposition velocities for MIC might be expected to be in the range 2-4 cm/s (Hicks, 1985). Taking V_d = 2 cm/s, and h=30 m, the dry deposition removal rate is estimated as

$$k_d = 6.7 \times 10^{-4}\ s^{-1} \tag{8}$$

which is comparable to the chemical removal rate.

Analytical solution of Eq.(3), subject to the initial and boundary conditions, is obtained by the method of integral Fourier transforms. In order to facilitate practical application of this solution, the eddy diffusivities D_y and D_z are expressed in terms of the semi-empirical plume dispersion parameters, σ_y and σ_z, as follows:

$$\sigma_y^2 = 2\, D_y\, x/U \quad , \quad \sigma_z^2 = 2\, D_z\, x/U \tag{9}$$

The final expression can be written as

$$C(x,y,z,t) = \frac{Q(t)}{\sqrt{2\pi}\, U\, H\, \sigma_y} \exp\left\{- \frac{y^2}{2\sigma_y^2} - k_t \frac{x}{U}\right\}$$

$$\cdot \left[1 + 2 \sum_{n=1}^{\infty} \cos\left(\frac{n\pi z}{H}\right) \cos\left(\frac{n\pi h_s}{H}\right) \exp \left\{-\left(\frac{n\pi\sigma_z}{H}\right)^2 \right\} \right] \tag{10}$$

A computer program was developed and run on the ICL 2960 system at IIT, Delhi. The wind speed at the effective stack height was estimated by the power-law profile from the wind speed (3 m/s) at 10 m height, using an exponent value of p = 0.35 for stable conditions. The wind direction and mixing height H were specified as discussed in Section 2. The spreads, σ_y and σ_z, were given by Briggs'(1973) urban curves for stability classes E-F. The stack inside diameter was 0.2 m, and the estimated gas exit-velocity was 88 m/s. The effective release height h_s was estimated to be about 40 m from simple plume rise calculations (e.g., Holland, 1953) under stable conditions.

Figure 3 shows the variation of the ground-level concentrations (GLC) as a function of downwind distance along the plume centerline after 45 min of time integration. The model simulation results are given in Table 4, which lists the total time-integrated GLC, surface deposition fluxes, and the approximate times of initial impact (i.e., plume front arrival) at the various affected sites. These sites are marked in Figure 4 which shows the concentration contours demarcating various zones of the affected areas based on the estimated total GLC. In general, the estimated GLC distribution and the plume arrival times seem to correlate well with the extent of affliction at the various sites and information obtained from interviews with survivors.

It is clear (from Fig. 4) that within zone I, encompassing sites 1-3, extremely high concentrations of the gas prevailed. The calculated maximum GLC were greater than 50 ppm. According to local residents, these colonies were engulfed by copious dense white fumes with a bitter sweet smell; visibility was very low. These were also the worst affected areas, with total mortalities adding up to 360 (out of a population of 6,173) by the time the smoky pall lifted at 5:30 am. The major medical symptoms in the survivors were severe eye irritation, coughing, vomiting, and excruciating chest pain. Zone II, which includes sites 4-6, was also a very badly affected zone. Here the estimated GLC were above 15 ppm. About 508 casualties were reported within this area (the toll was higher in this zone since it includes many more colonies with a much larger population than zone I). About 87% of the initially recorded casualties were within these two zones. Model results (Table 4) suggest that the plume front arrived at these sites within the first 6 min of the episode.

Zone III, the "zone of moderate effects", encompassed sites 7-11, 14, 22, and 23. The immediate fatalities were 11, much lower than in zones I and II. People experienced severe eye irritation and breathing difficulties. The estimated gas concentrations in this zone were between 15 and 1.5 ppm. Zone IV, encompassing sites 12, 13, 15-21, and 24-26, is the "zone of marginal effects" with only five fatalities. The estimated concentrations here were less than 1 ppm. Some residents experienced slight eye and throat irritation, though no traces of the fumes were visible. As described earlier, many people fled their homes during the episode and, hence, there is an inherent subjectivity involved in this correlation study. However, many of the casualties occured close to their normal place of residence. The effects of the gas faded significantly with increasing downwind distance. Though humans and animals inhabiting the region extending out to 6 km downwind of the plant were affected by the gas, the heaviest toll occured within the first 200 m to 1 km distance.

Table 4. Model Estimates of GLC and Deposition Fluxes of MIC.

Site	GLC (ppm)	Surface Deposition Flux (μg/m2/s)	Time of Initial Impact (min)
1	93.5	4133	1.2
2	74.2	3280	1.6
3	57.4	2537	1.6
4	25.9	1145	3.9
5	18.5	818	5.4
6	15.5	685	5.8
7	8.0	354	8.6
8	3.4	150	10.9
9	2.5	111	13.7
10	8.2	362	49.7
11	8.6	380	50.4
12	0.1	5	51.6
13	0.2	9	57.4
14	1.7	76	57.4
15	0.9	39	58.6
16	1.0	43	60.1
17	0.4	18	61.3
18	1.0	44	61.7
19	0.3	13	61.7
20	0.6	26	63.6
21	0.2	9	63.6
22	3.4	150	78.9
23	1.8	80	80.8
24	1.0	44	82.8
25	0.8	35	82.8
26	0.7	30	85.2

This agrees with the calculated downwind variation of the GLC (see Fig. 3). The total of early fatalities listed above is rather low by present estimates, since many of the deaths were not recorded.

The best concentration monitors available in the Bhopal gas disaster were the affected trees, plants, crops, and soil, which were studied by Indian scientific organizations. The imprint of the toxic gas could be discerned on all types of vegetation including tall trees, shrubs, and ground-level crops. Vegetable and spice crops were most affected in the eastern, southeastern, and southern directions from the factory. Some vegetation looked as if it had been burned. It was observed that the same species of plants, which were badly damaged by the gas in other areas, were mostly unaffected near the water. Also, the same species of crops showed relatively less damage in fields which were irrigated on the evening preceding the accident. This could be due to the great affinity of MIC to water and its rapid hydrolysis resulting from the increased moisture content in the soil, vegetation, and surface air. Some of the large trees were totally defoliated, while others showed acute to mild effects, depending on the species and location relative to the factory. Table 5 shows the extent of the vegetation damage in terms of area. These vegetation

Table 5. Classification of Vegetation Damage Due to Exposure to the Toxic Gases.

Zone	Classification	Area (km^2)
A	Severely affected	3.5
B	Badly affected	10
C	Moderately affected	6
D	Mildly affected	5

damage zones, shown in Figure 5, indicate that trees and vegetation within zones A, B and C could indeed be affected by exposure to the spreading gas, with estimated concentrations ranging from very high to moderate values. Zones A and B correspond reasonably well to zones I, II, and III shown in Fig. 4. The vegetation-damage contours are also tilted towards the SE, similar to the concentration contours.

MEDICAL CARE, RELIEF, AND REHABILITATION

Inhalation of MIC, mixed initially with unknown amounts of other poisonous gases (see Table 3) from the leak, is considered to have resulted in the large number of deaths in humans and animals. The initial symptoms displayed by the survivors were burning sensation in eyes, nose and throat, breathing difficulty, coughing, vomiting, headache, lethargy, and disorientation. The main target organs were the eyes and the lungs. Lung damage was the cause of death in most of the casualties.

While vision and condition of the injured eyes have dramatically improved following medical treatment, lung problems persist in many victims. Pulmonary edema resulting from the exposure to MIC gas was treated with steroids, bronchodilators, oxygen, and antibiotics; a large number of patients have recovered. However, many of the survivors were left with considerable damage to their small airways and alveoli. The worst affected among this group were children. About 39% of the patients showed moderate to severe pulmonary disability. Those who display normal functional status may still have significant lung pathology. Open lung biopsy performed in some of the severely affected patients has led to the detection of bronchiotitis obliterans and interstitial fibrosis. Attempts are being made to identify lesions in victims in the early stages, and treat them using drugs and physiotherapy.

Miscarriages and stillbirths were frequent to the approximately 3000 pregnant women who were exposed to the gases. In the first 20 weeks, 436 spontaneous abortions occurred out of 2600 pregnancies; the normal rate for Bhopal was 6 to 10%. Gynecological disorders in various forms were reported in a large percentage of the women exposed to the gases.

Cyanide poisoning in the survivors resulted from direct exposure to HCN gas, during the first hours in the areas closest to the plant, as well as indirect exposure owing to unusual generation of toxic amounts of cyanide in the body after exposure to MIC. Some experts believe that the "cyanogen pool" resulting from the latter can persist in the human body for a very long time. The Indian Council of Medical Research (ICMR) studied this controversial issue, and recommended continued treatment of symptomatic patients with sodium thiosulfate, the antidote for cyanide poisoning, under careful medical supervision.

The state government has opened 16 dispensaries, a new 30-bed hospital with modern equipment, and 25 mobile clinics in the affected areas, in order to provide effective medical care to the Bhopal gas victims. A 60-bed ward and MIC clinic, equipped with a computerized blood gas analyzer, was established in the Medical College Hospital to undertake various sophisticated investigations and develop the best methods of treatment. In addition, 100 more beds were reserved exclusively for the gas victims in other hospitals in Bhopal. Disaster relief measures undertaken by the government include financial assistance to affected families, cash grants to low income group victims, free rations of essential commodities, and supplies of nutritious food to pregnant women, lactating mothers, and infants. A comprehensive rehabilitation plan consisting of housing and urban development, vocational training and employment schemes, and establishment of work centers and community facilities, is being implemented in the affected areas. Many voluntary organizations are supplementing the government efforts in medical care and rehabilitation.

Numerous studies on the Bhopal gas disaster have been carried out in India, and many others are still in progress at various government laboratories, universities, medical colleges, and hospitals. The biomedical and toxicological studies on the long-term effects of MIC gas on the survivors are being coordinated by the ICMR. The Council of Scientific and Industrial Research is coordinating the scientific and technical projects. Various issues raised by the Bhopal tragedy (such as development policy, industrial hazards and public safety, occupational health, environmental protection, legislation, and other topics) are being studied and addressed by a number of government agencies, and by scientific and public interest groups. The Central Insecticides Board has banned the use of 25 highly toxic pesticides, including the two MIC-based products, Sevin and Temik.

CONCLUSIONS

The most important legacy of the Bhopal tragedy is its enormous worldwide impact in raising the level of public awareness and concern over the hazards of chemical plants to the general public, especially in those plants involving toxic chemicals. This will inevitably generate change in safety procedures, equipment to prevent and contain toxic releases, and the kind of information given to the public about chemical hazards. Most chemical companies have perceived the need to reassure the public of the safety of their operations after Bhopal.

The Bhopal disaster bears many important lessons of immediate global relevance, which can be briefly summarized as follows:

(1) Information: Industries with potentially dangerous processes should work together with state and local officials to maintain a current understanding of what they are doing, giving details of the toxic substances, potential hazards, toxicological effects, medical treatment, and other pertinent information.

(2) Industrial siting and urban planning: Hazardous industries should be located far away from population centers with due regard to potential impacts on the total environment. Existing chemical plants in urban areas should be relocated, if possible, or isolated from dense residential areas by a 2-3 km radius green buffer zone planted with sensitive tree and vegetation species to act as chemical monitors.

(3) Standards and enforcement: Industrial safety, worker and community health, and environmental regulatory standards appropriate for each industry should be established and strictly enforced. Regulatory agencies should carry out frequent inspections of hazardous plants to examine the safety of processes and equipment, and to verify compliance with regulations.

(4) Emergency response: This consists of several components. The scientific program should address atmospheric behavior of toxic chemicals including transport, dispersion, transformation, and deposition, ultilizing appropriate models and monitoring. The medical response should require that hospitals and physicians be knowledgeable about the toxicology and treatment for exposure to locally used toxic chemicals, and should be prepared to handle any emergency. The state and local authorities, in cooperation with the concerned plant, should develop effective communications, evacuation plans, and community education programs.

(5) Management: The management of chemical companies at all levels, in view of their responsibilities for industrial and public safety, should play a leading and constructive role in most of the areas listed above, especially in providing information and developing appropriate emergency response programs. Procedures involving the manufacture, storage, transportation, and disposal of toxic chemicals should be periodically reviewed to minimize potential hazards to public health and safety. Worker training and plant safety audit programs should be intensified.

Bhopal holds out lessons that have to do with social responsibilities of science and technology, and basic human concerns for safety, for standards, and for good common sense. If these lessons are lost, then it is all too possible that accidents such as this may be repeated in another factory in another city in another way. A fitting memorial to the victims of the Bhopal Gas Tragedy would be to make sure that this shall not happen again.

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DISCLAIMER

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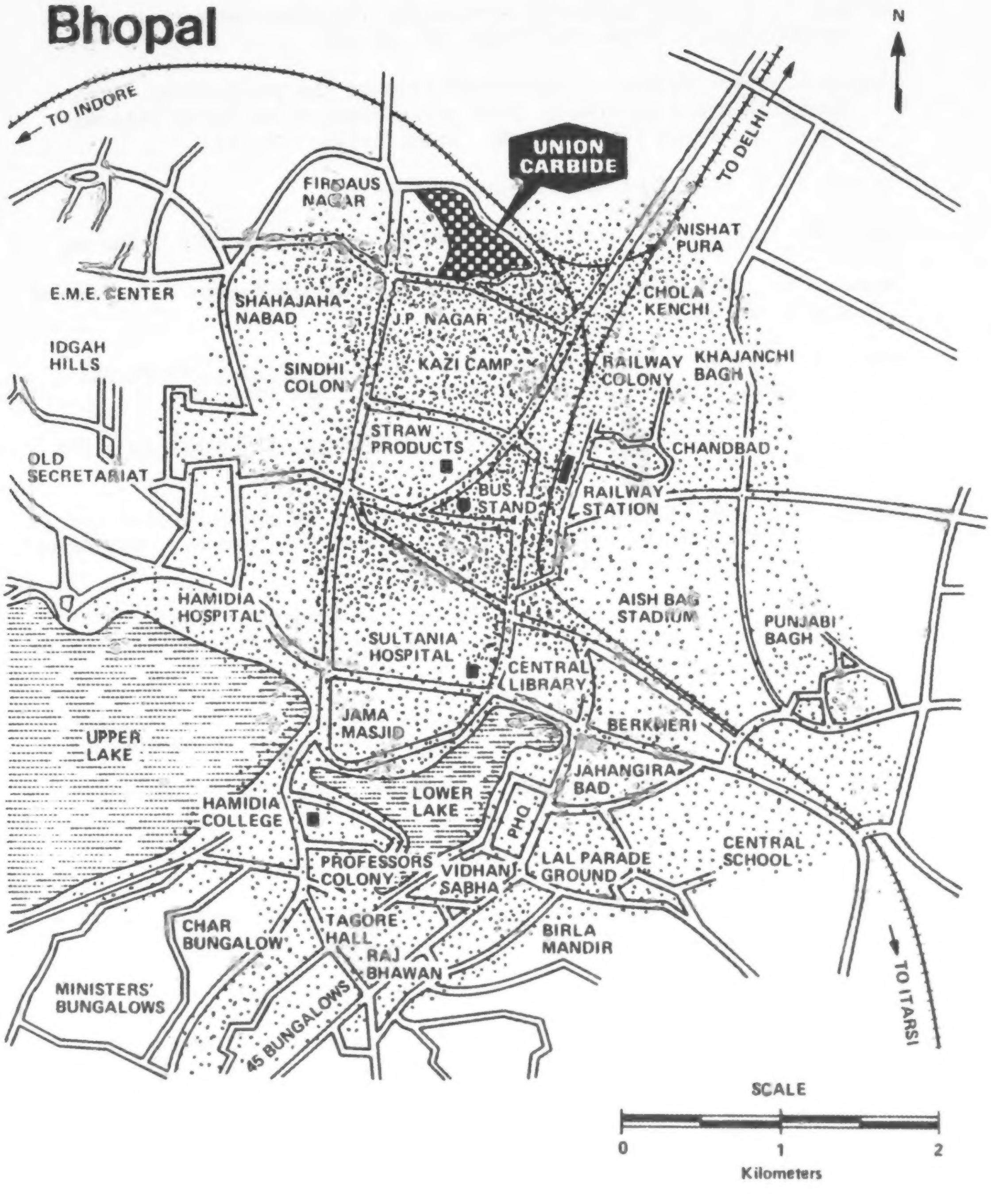

Figure 1. A partial map of Bhopal showing the location of the UCIL pesticide plant and its environs. The dotted area shows the localities affected by the toxic gases.

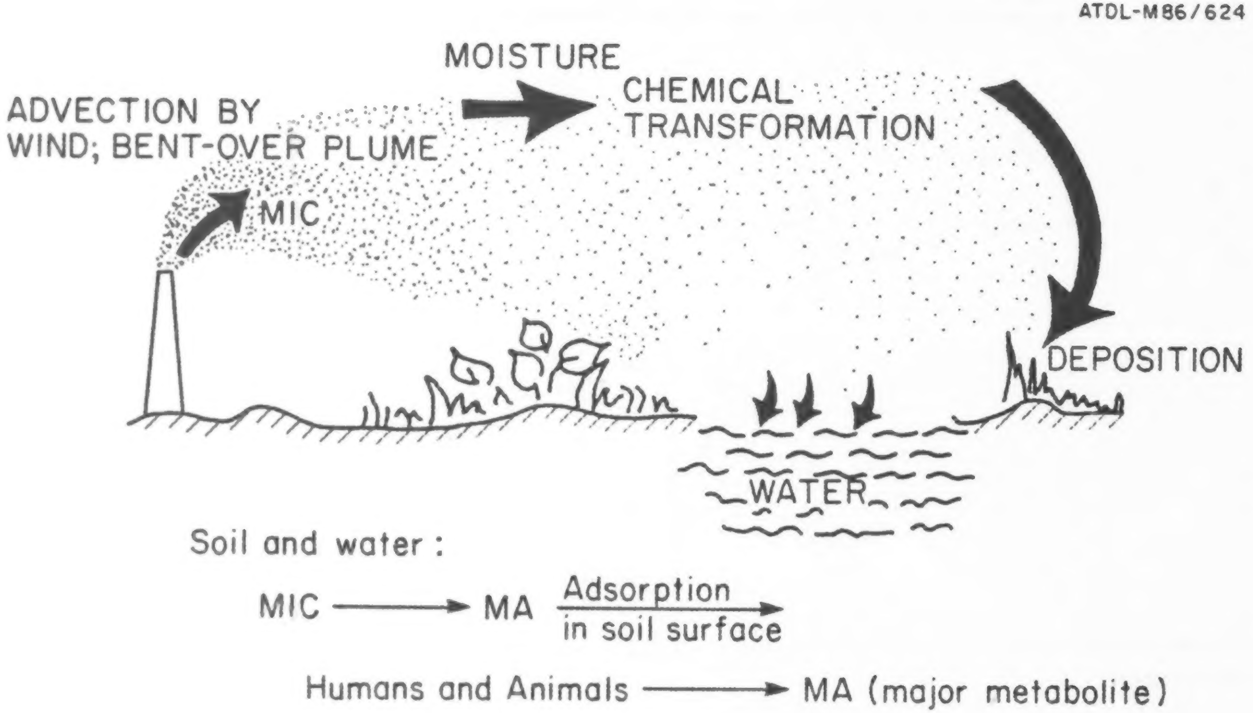
ATDL-M86/624
ADVECTION BY WIND; BENT-OVER PLUME
MIC
MOISTURE
CHEMICAL TRANSFORMATION
DEPOSITION
WATER
Soil and water :
MIC ⟶ MA ⟶ Adsorption in soil surface
Humans and Animals ⟶ MA (major metabolite)

Figure 2. A schematic diagram showing the atmospheric behavior and fate of MIC plume in the environment. Methylamine (MA) is the major product of MIC reactions in soil and water.

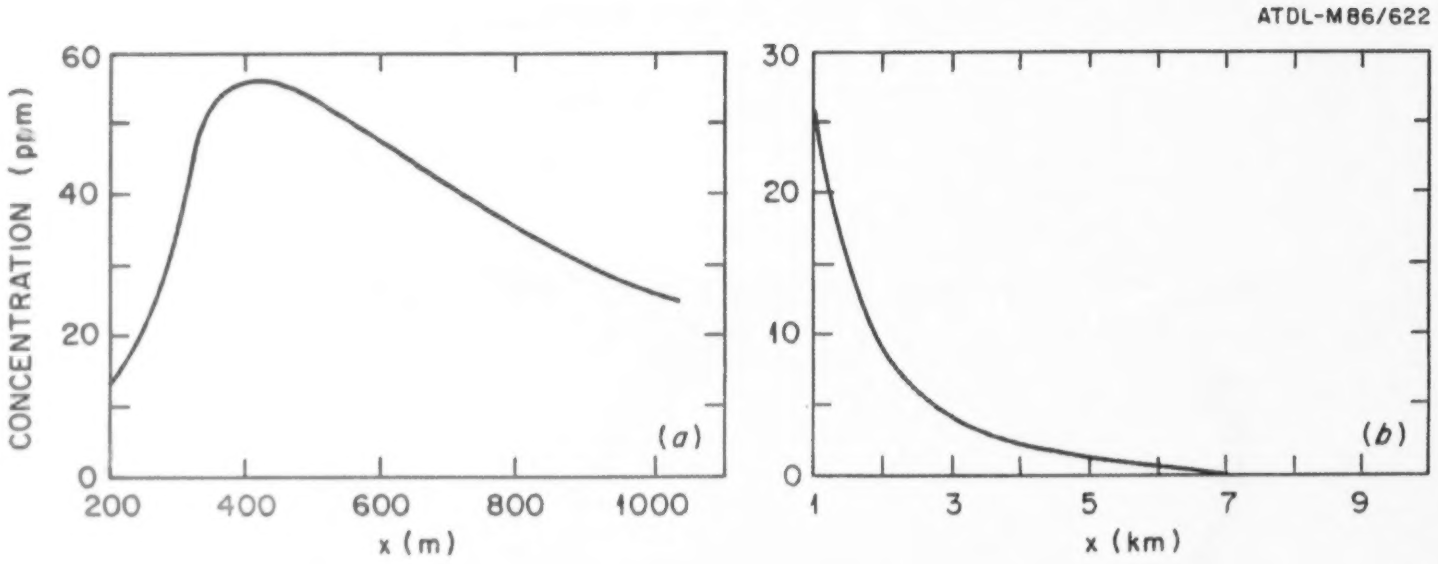

Figure 3. Variation of the estimated ground-level MIC concentrations as a function of downwind distance along the plume centerline after 45 min of time integration: (a) near field, (b) far field.

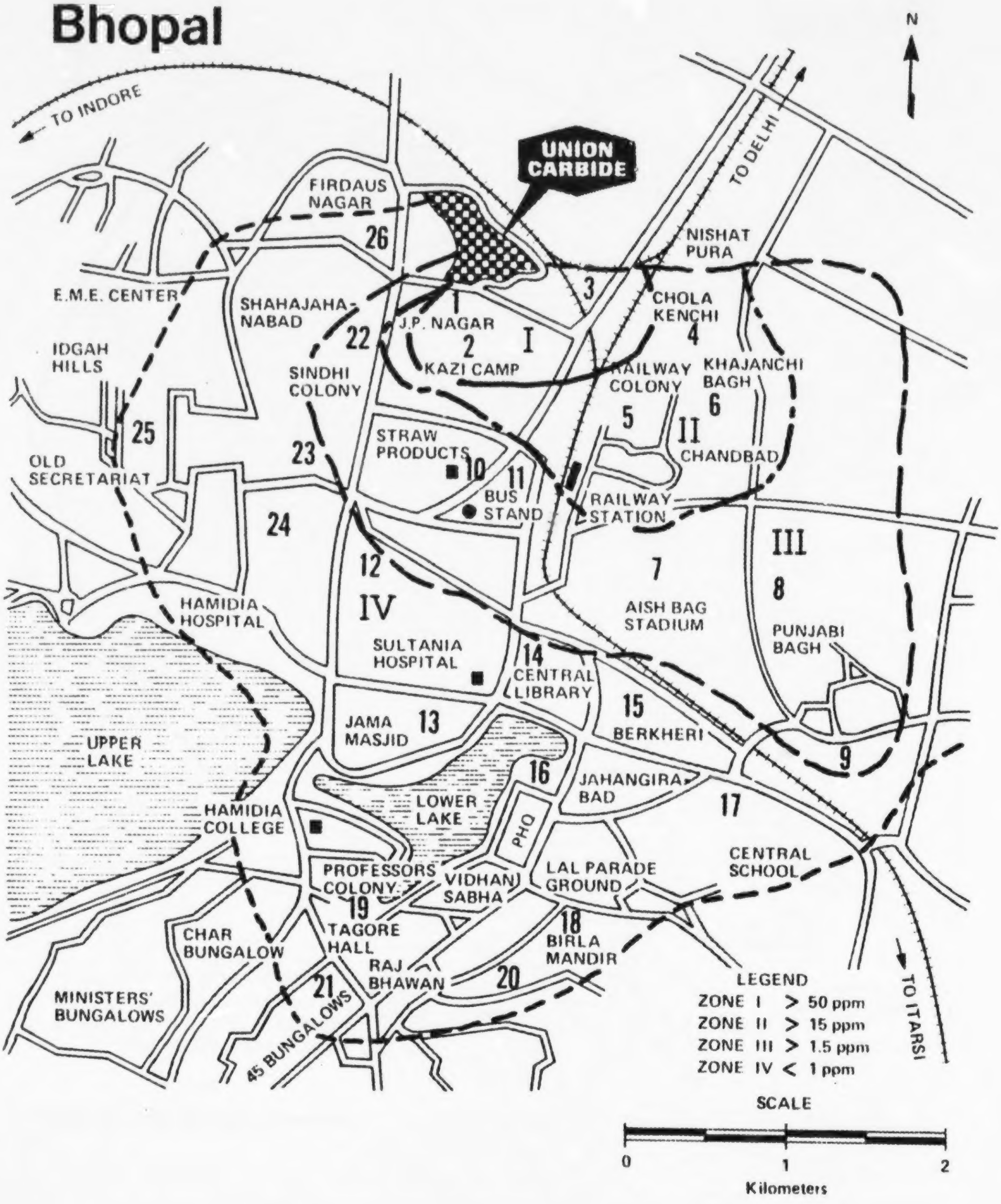

Figure 4. Modeled concentration contours demarcating the various zones of the gas affected areas based on the estimated GLC. The numbers 1-26 denote the localities in Bhopal affected by the gas leak, where the GLC are specifically calculated and given in Table 4.

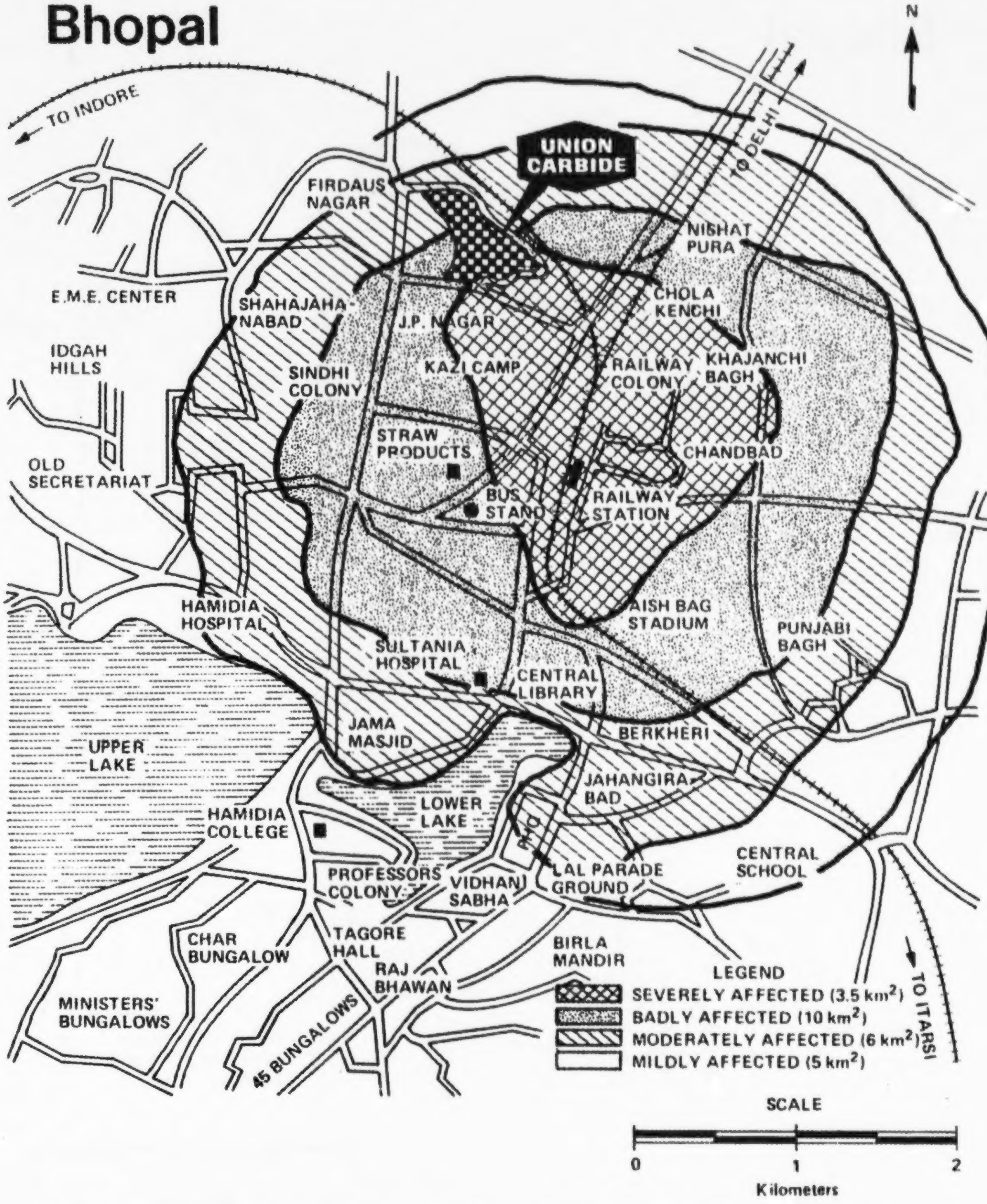

Figure 5. Vegetation damage contours demarcating the various zones of injury to plants by the toxic gases. These contours are based on a detailed survey of vegetation and crops in Bhopal conducted by the Indian Agricultural Research Institute and the Central Board for Prevention and Control of Pollution, following the gas leak.

APPENDIX B

On the Development of Reactive, Dense Gas Models

On the Development of Reactive, Dense Gas Models*

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ABSTRACT

Chemical reactions between released pollutants and atmospheric constituents can influence atmospheric dispersion if the heats of reaction are such that buoyancy can be affected or mechanical turbulence damped. If the reaction is sufficiently exothermic, plume rise can be increased; if sufficiently endothermic, then plume rise can be suppressed. It is necessary to consider the potential influence of such reactions on the mixing rates characteristic of the ambient air. Reaction rates are also a critical issue. If reactions are completed rapidly, then in concept it is possible to assimilate the consequences of the reactions in the source term initialization or in the first time step of a numerical model. On the other hand, if reaction rates are slow in comparison with the time step of a simple model, then a more complicated and detailed modeling effort may be required.

1. INTRODUCTION

The wide variety of needs for numerical models of atmospheric dispersion imposes requirements for models of a wide range of complexities. It is clear that simple models giving conservative estimates are most suitable for purposes of real-time emergency response, whereas more sophisticated models can be used for assessment of risk, for planning response strategies, or for evaluation of the consequences of previous accidents. The range of modeling capabilities must also be adequate to encompass the spectrum of circumstances to be addressed, involving terrain complexity, different meteorological conditions, and source configurations.

In general, the complexity of the model best suited in some special application is increased by increasing complexity of the circumstance and limited by the time interval available in which to run the model. Considerable additional complexity can arise if the pollutant involved is dense, or if it reacts chemically after emission. The case of dense gas dispersion has received extensive attention, largely as a result of problems associated with the transport and storage of liquified gaseous fuels. In essence, the density interface is a stabilizing influence, tending to isolate the underlying "bubble" of dense gas from the turbulence of the ambient atmosphere. The volume of dense gas itself can then be free (if dense enough) to respond to its own dynamical forces, largely independent of the atmosphere passing over it. Spreading may be rapid, but dilution may be correspondingly slow.

Endothermic chemical reactions impose a further set of complications, that can serve to make a pool of emitted trace gas act as if it were a genuine dense gas, even though quite dilute. On the other hand, some chemical reactions are exothermic, and will tend to increase vertical mixing between the trace gas and the ambient air.

The present purpose is to explore the options available to modelers faced with the need to consider the consequences of exothermic and endothermic reactions. We start with the assumption that a suitable modeling framework is available, including dense-gas formulations appropriate to the case under consideration, with which chemically-induced dynamic factors must then be combined.

2. SOME THEORETICAL CONSIDERATIONS

Consider a trace gas released into the air and reacting with some atmospheric constituent, such as atmospheric water vapor. The chemical reaction is then of the general type

$$X_1 + H_2O \xrightarrow{k_c} X_2 + X_3 + J \qquad (1)$$

where species X_1 reacts with H_2O (in this example) to form species X_2 and X_3 with rate constant k_c (s^{-1}) and releasing thermal energy J (Joules $mole^{-1}$). If J is positive, then the reaction enhances the mixing due to buoyancy. In this case, it is informative to consider the role of the additional thermal energy in the context of related features of the ambient air.

In a convective atmosphere with sensible heat flux H, the rate of generation of turbulent energy associated with the heat flux is

$$\Pi_B = (H/c_p).(g/\theta) \qquad (2)$$

where c_p is the specific heat of air at constant pressure, g is the acceleration due to gravity, and θ is potential temperature (absolute). The equivalent mechanical term is

$$\Pi_M = -\tau \cdot (\partial u/\partial z), \tag{3}$$

where τ is the surface momentum flux and $\partial u/\partial z$ is the local wind gradient at the height in question. The negative sign is a consequence of the sign convention, with positive τ being directed away from the surface and $\partial u/\partial z$ positive when wind increases with height.

In classical micrometeorology, the importance of buoyancy relative to shear-produced mechanical diffusion is quantified by the ratio of (2) to (3):

$$\begin{aligned} \zeta &= -(gH/c_p\theta)/(\tau \cdot \partial u/\partial z) \\ &= [kzgH/(\rho c_p u_*{}^3\theta)]\ \phi_m{}^{-1} \\ &= (z/L).\phi_m{}^{-1} \end{aligned} \tag{4}$$

Here, standard micrometeorological relations have been invoked to relate the local wind gradient and shear stress to the friction velocity, u_*, involving air density ρ and height z, and introducing the von Karman constant k and the stability-dependent dimensionless wind shear ϕ_m. The quantity L is the Monin-Obukhov length scale of turbulence, initially derived from dimensional arguments. The quantity ζ is thus an index of dynamic instability associated with buoyancy, much like the familiar index z/L.

In this context, it is useful to consider a second buoyancy term, like Π_B, but representing the consequences of an exothermic chemical reaction.

$$\Pi_C = k_C J \rho_v / M_v \qquad (5)$$

where ρ_v is the partial density of the species X_1 in air (kg m^{-3}) and M_v (kg $mole^{-1}$) is the molecular weight of the species X_1.

It is then apparent that if the ratio

$$\begin{aligned} \zeta_B &= \Pi_C/\Pi_B \\ &= k_C J \rho_v c_p \theta/(HgM_v) \end{aligned} \qquad (6)$$

is large (with respect to unity, then the reaction is sufficiently exothermic to modify buoyancy significantly, in unstable conditions.

In unstable stratification, an endothermic reaction will tend to reduce the rate of buoyant mixing. In general, therefore, a modified index of the net effective instability can be postulated:

$$-\zeta' = (\Pi_B + \Pi_C)/\Pi_M \qquad (7)$$

where Π_C is positive for an exothermic reaction (positive J) and negative for endothermic.

Although the modified stability index ζ' has been developed here for unstable conditions, its generality is not so constrained. Just as z/L and Ri are stability indices that extend across the range of stable and unstable stratification, so does ζ' provide an equivalent mechanism for modifying such standard quantities in the cases of exothermic and endothermic chemical reactions.

Equations (6) and (7) provide a basis for "screening" chemical reactions for potential concerns related to modifying atmospheric mixing. Consideration of dense-gas effects can be included in the same general framework. In this case, consideration of relevant time scales provides useful physical insight. At a density interface, characterized by a difference $\Delta\rho$, the restoring force (per unit volume) associated with the displacement of a unit volume of denser fluid into the (upper) less-dense medium is

$$F_r = g.\Delta\rho \tag{8}$$

A time scale (T_d) associated with relaxation of the displaced parcel is then

$$\begin{aligned} T_d &= (\rho.\Delta z/(g.\Delta\rho))^{1/2} \\ &= (\rho.\Delta z/(g(\rho_v-\rho)))^{1/2} \end{aligned} \tag{9}$$

This is like the time scales associated with restoration of a displaced air parcel in ambient stratification:

$$T_b = ((\theta/g)/(\partial\theta/\partial z))^{1/2} . \tag{10}$$

the inverse of which is the familiar Brunt-Vaisala frequency. The mechanical term that arises in related contexts is the time scale associated with the wind shear,

$$T_M = (\partial u/\partial z)^{-1} \tag{11}$$

Standard considerations of T_b and T_M lead to the generation of the gradient Richardson number,

$$Ri = (T_M/T_b)^2 \tag{12}$$

A suitably modified form which includes effects of density gradients might then be constructed as

$$Ri = T_M^{\,2}\cdot(T_b^{\,-2} + T_d^{\,-2}). \tag{13}$$

Inspection of this further modification is not especially revealing, since it is no more than a restatement of the observation that local density variations must be used to correct ambient stratification calculations when considering local stability. Such matters have been dealt with extensively elsewhere.

3. DISCUSSION

Inspection of the relations involving J reveals a few hidden difficulties. In particular, the chemical reaction rate k_c is not usually a constant, but depends on variables which might include temperature, pressure, and solar radiation. Furthermore, the reaction may be equivalent to a gas-phase titration, in which the reaction is controlled by the rate of delivery of one gaseous reactant or the other. Thus, from the present viewpoint the specification of k_c is far from trivial.

Inspection of equations (6) and (7) reveals several intriguing conclusions.

(a) Plume rise enhancement/suppression

- The practical effect of the release of heat of reaction is likely to be greatest in near-neutral conditions (when H is small). The diurnal cycle of H is large, such that H varies from -10 to -20 W m^{-2} at night to more than 200 W m^{-2} at midday, typically. The influence of J is therefore likely to be greatest near dawn and dusk.

(b) Mechanical mixing with the ambient air

- The suppression of dilution by an endothermic reaction is a strong function of the friction velocity, suggesting an inverse cubic dependence on wind speed.

- The roughness of the surrounding surface is important, insofar as it controls u_* in given wind speed conditions. Minimum boundary dilution rates will occur in light winds, over smooth terrain.

(c) The role of the reaction rate

- The reaction rate enters as a first-order factor in both ζ_B and ζ_M. The appropriate reaction rate is the effective value in the conditions of interest, which will generally be less than the rate based on chemical consideration alone. The problem that arises is associated with turbulent mixing; chemical reaction consumes material available in any specific volume, and hence the rate of resupply of reactions must be considered. Thus, if the rates k_C in equations (6) and (7) are based on chemistry alone, then the properties ζ_B and ζ_M should be considered as indices of the potential importance of the heat of reaction, rather than an indication of actual importance in any specific instance.

4. A PRACTICAL APPROACH

The need to consider the special characteristics of reactive gases in dispersion models leads immediately to two fundamental questions:

(a) Does the reaction cause the dynamic behavior of the atmosphere to be modified?

(b) Is the reaction completed fast enough that the consequences can be accommodated in the source term of a relatively standard dispersion code, or in its first time step?

The answers to those questions will determine the complexity of the model which must then be used. In some instances, such as when a reaction is strongly exothermic yet quite slow, a complicated model is likely to be required in all situations, and the need for rapid computation as for real-time emergency response are unlikely to be realized.

An objective approach is to use a detailed simulation of the chemistry to derive the necessary answers concerning reaction rates and exothermicity in natural conditions. If the results of these explorations are satisfactory, then perhaps simpler models can be designed without loss of either generality or applicability.

This general philosophy is presently being tested in the development of a model of dispersion of uranium hexafluoride. This material is used in uranium processing and isotopic enrichment. Upon release into the atmosphere, it reacts exothermically with water vapor, generating particulate uranyl fluoride and gaseous hydrogen fluoride. The amount of heat released and the rapidity of the reaction are clearly dependent on ambient humidity. In this instance, consideration of scaling properties such as were discussed above is not completely satisfying, since factors not included in the development of the scaling properties might be critical.

The chemical reaction is as follows:

$$UF_6 + 2H_2O \longrightarrow UO_2F_2 + 4HF + J. \qquad (14)$$

The quantity J is a function of temperature and pressure, but in typical conditions involving gaseous UF_6 and water vapor, $J \simeq 5.86 \times 10^4$ kJ/kg based on chemical considerations alone (see summary by Just et al., 1985).

A sophisticated numerical model of UF6 reactions in air was developed earlier (Just, et al., 1985). This includes a detailed description of the turbulent resupply of reactants as material is consumed (Varma, 1982), and provides a convenient tool for investigating the rapidity of UF_6 reactions in air. Figures 1 and 2 illustrate the results. In Figure 1, the reaction rate is seen to be short in comparison to the time step of typical puff-dispersion models (usually about five minutes), except for very dry conditions. Figure 2 shows that there is little need to consider background atmospheric stability as a controlling factor, since in even the most stable case considered the reaction appears to be completed in 30 seconds. Hence, in this particular case it appears adequate to assimilate the chemistry and its consequences in the first time step of a standard puff model, and to use the more detailed chemical model to initialize the chemically-simpler scheme.

5. CONCLUSIONS

Two major questions arise when adding chemical reactions into an existing dispersion scheme (either of possible trace gases or dense gas). First, the rapidity of the reactions must be considered. If the reactions are completed quickly in comparison with the time step of the model under consideration, then the relevant chemical reactions can be accommodated within the initial time step, or perhaps assimilated in the specification of the source term.

Second, consideration must be given to the consequences of the heat of reaction. If exothermic, the reaction is essentially a destabilizing factor, working to increase plume rise and to enhance buoyant mixing (and subsequent dilution rates).

If endothermic, the reaction is essentially a stabilizing influence, increasing local stratification, and hence decreasing mixing (and dilution) rates. If all other factors are equal, a bubble of endothermic material must maintain its integrity for a longer time than a bubble of exothermic material.

An examination of these factors can be based either on first principles, by consideration of the relative magnitudes of the dynamic effects of the heat of reaction, or on the use of a detailed model. In practice, if the reaction involves a trace gas constituent of the ambient atmosphere (e.g., H_2O or CO_2), then the use of a detailed chemical model appears especially beneficial. In such cases, the reaction can proceed as a gas-phase titration in which the rates involved and the thermodynamic consequences are controlled by the rates at which reactant gases are fed to the reacting volume.

6. REFERENCES

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Varma, A. K., 1982: Development of models for the analysis of atmospheric Releases of Pressurized Uranium Hexafluoride," ARAP Report No. 482, Aeronautical Research Associates of Princeton, Inc., Princeton, NJ.

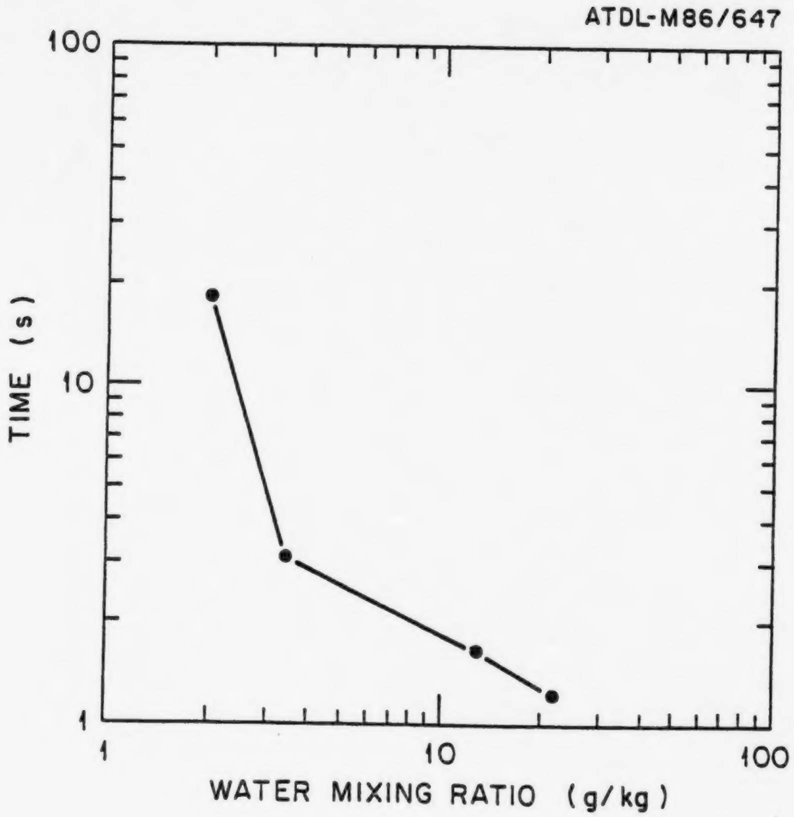

Figure 1. The humidity dependence of the exponential time scale of reaction of UF_6 released into air, as computed by a sophisticated chemistry/turbulence mixing model (Just and Williams, 1985). Time scales correspond to (1-1/e) completion of the reaction.

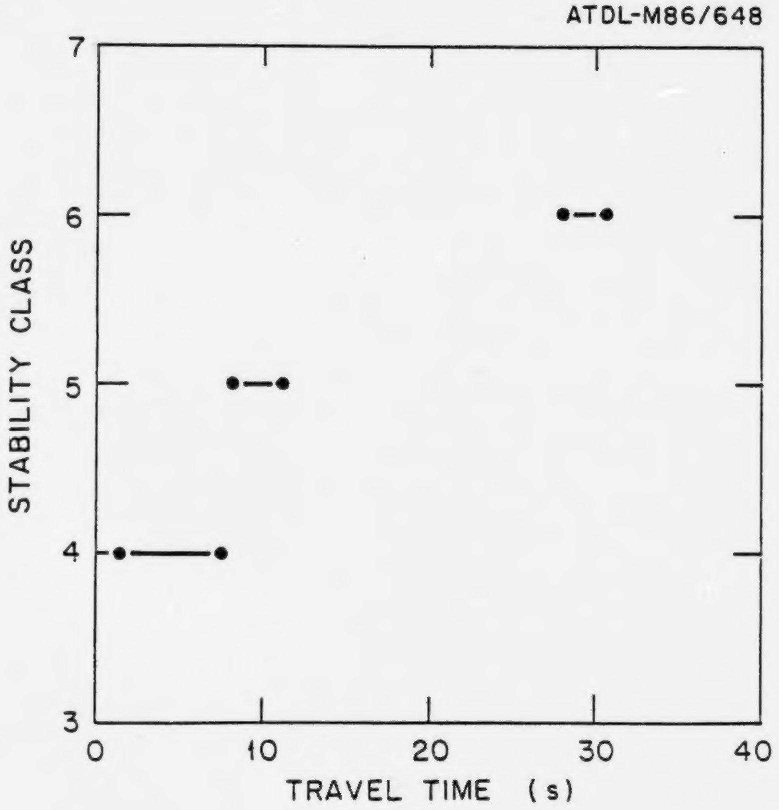

Figure 2. The dependence on stability class of the exponential characteristic time scale, as plotted in Figure 1.

APPENDIX C

Mathematical Models for Atmospheric Dispersion of Hazardous Chemical Gas Releases: An Overview*

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*Presented at the AIChE Center for Chemical Process Safety, International Symposium on Preventing Major Chemical Accidents, February 3-5, 1987, Washington, DC.

MATHEMATICAL MODELS FOR ATMOSPHERIC DISPERSION OF HAZARDOUS CHEMICAL GAS RELEASES: AN OVERVIEW

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Mathematical models are required for prediction of atmospheric dispersion of heavier-than-air gases to assess hazards of unconfined vapor cloud combustion and toxicity. The dispersion process involves three more-or-less distinct regimes of fluid flow: buoyancy-dominated, stably stratified, and passive dispersion. For releases on uniform terrain, similarity models are available for the description of all three regimes with sufficient accuracy for most risk assessment and emergency response requirements. 3-D mathematical models can, in principle, simulate the spatial and temporal dispersion process without artificial separation of the flow into separate regimes and may be able to provide for effects of terrain and wake turbulence. Evaluation of 3-D models is underway, but most of the work is biased strongly toward evaluation against data for dispersion in the absence of terrain and wake turbulence effects, even though description of these effects is a primary motivation for their use. Future research should be directed to the verification of models which provide for the effects of terrain and wake turbulence, and for description of jetting releases, aerosol formation, chemical reaction, and deposition.

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INTRODUCTION

The recent accidents at Bhopal and Mexico City illustrate the potential dangers of acutely toxic or combustible gas clouds. These catastrophes have intensified pressures on Government to "do something" about major industrial accidents. The European Community's Seveso Directive calls for tighter regulatory controls to reduce the likelihood and consequences of "major hazards", and the response has been to implement tighter regulations of activities using hazardous chemicals. The regulations require provision of evidence that hazards to man and the environment have been identified and that suitable precautions have been taken to minimize occurrence and potential consequences. Many chemical manufacturing, storage, and transportation activities with large inventories of hazardous materials have had specific requirements imposed, including

- submission of safety assessments
- preparation of on-site emergency response plans
- preparation, in cooperation with the local authorities, of off-site emergency plans
- provision of information to people in the vicinity who might be affected by a major accident

Pressures for similar regulatory controls are increasing in the United States.

The concept of separation distances, by which the consequences of major accidents are ameliorated, is implicit in regulations being considered world-wide. Methods are required for prediction of atmospheric dispersion of hazardous gas releases, of which the main hazards are vapor cloud combustion and acute toxicity, to aid in the determination of appropriate separation distances. Separation distances are required for siting fixed hazardous chemicals operations, and for the preparation of emergency response plans. Methods are also required for predicting atmospheric gas dispersion in support of emergency response to transportation accidents.

Prediction of separation distances for use in risk assessment and emergency response is controversial. The inclusion of this review of mathematical models for atmospheric dispersion of hazardous chemical gas releases, and lesser consideration of modeling methods applicable to predicting other accident phenomena such as fire/explosion damage or toxicity effects, indicates the importance attached to this question by the chemical industry and regulatory parties. The Environmental Protection Agency and Department of Energy jointly sponsored a "Workshop on Determination of Atmospheric Dilution for Emergency Preparedness" in October 1986 with the following principal objectives.

- to review current methods for determining release characteristics, source strength, and dispersion of hazardous gases released into the atmosphere for use in hazard evaluation and emergency response
- to provide recommendations for choosing among the current methods for immediate use
- to assess the specific strengths and weaknesses of available methods and make recommendations for their improvement.

The controversy can be traced to predictions in the mid-70's of the extent of the hazard zone around an accidental release of liquefied natural gas (1). A postulated accident of concern was the rupture of one or more 25,000 cubic meter LNG ship cargo tanks. Since the vapor cloud which would be formed following the spillage of such a large quantity of LNG onto water would be cold, it would be expected to be significantly heavier than air. Air pollutant dispersion models (primarily Gaussian similarity models with ad hoc provision for gravity spreading of the heavy gas) were applied, with widely disparate results, to predict the extent of flammable gas-air mixtures from these "worst credible" releases (2). The disparity of such dispersion predictions made more uncertain the risks associated with LNG importation, and fostered an extensive research program aimed at better understanding the atmospheric dispersion of large quantities of heavy gases which are accidentally released.

Since van Ulden's proposal (3) of a simple mathematical model to describe the gravity spread and subsequent dispersion of a large volume of heavy gas instantaneously released into the atmosphere, there have been numerous other models proposed and extensive laboratory and field test experimental programs to provide data for model validation have been completed. Several recent reviews which describe the mathematical models are available (4,5,6). The field test programs completed at China Lake, California (7), Maplin Sands, England (8), Thorney Island, England (9), and Frenchman Flat, Nevada (10) to provide data for dispersion model validation have also been reported.

For dispersion scenarios where the gas cloud can be represented as having a regular shape, similarity mathematical models (such as the familiar Gaussian models in widespread use for passive atmospheric pollutant dispersion) are applicable. Similarity approximations are also justified for modeling accidental releases of large quantities of heavy chemical gases under certain conditions.

Complex (three-dimensional) mathematical models can, in principle, be used to simulate the spatial and temporal dispersion processes without the "artificial" separation of the flow into separate regimes required by the similarity models. Predictions can me made of dispersion effects due to nonuniform terrain and wake turbulence. It may also be possible to provide useful estimates of concentration fluctuations around the predicted mean (time average) values.

This paper reviews the mathematical modeling methods which have been developed for predicting atmospheric dispersion of hazardous chemical gas releases. The emphasis is on mathematical models for dispersion of heavier-than-air gases. Such emphasis is justified because the majority of hazardous chemical gases form heavy gas clouds following accidental release, and because such clouds remain near the ground for longer times and to greater distances.

PHENOMENOLOGY OF HEAVY GAS DISPERSION AND MODEL APPLICABILITY

The typical heavy gas dispersion process involves three more-or-less distinct regimes of fluid flow. Immediately following rapid release of a large quantity of heavy gas, a cloud having similar vertical and horizontal dimensions may form. Initial slumping and lateral spreading motion continues until the kinetic energy of the buoyancy driven flow is dissipated. As the dispersion proceeds, stable stratification due to the negative vertical density gradient decreases until the process can be represented as a neutrally buoyant plume (or cloud) embedded in the wind flow.

For heavy gas releases at ground level on uniform terrain with unobstructed wind each of the three flow regimes (buoyancy-dominated, stably stratified, and passive dispersion) can be approximated as a cloud (or plume) having a regular shape, and can be described with similarity models.

Similarity Models

When the cloud formation time t_f is very small compared to the time of cloud travel to the maximum distance exposed to the concentration of interest t_t, an "instantaneous puff" representation is applicable; if $t_f >> t_t$, a stationary "plume" representation of the cloud is indicated.

Figure 1 depicts the cloud shape which has been most frequently used in similarity heavy gas dispersion models for instantaneous releases. An initial volume of gas, usually

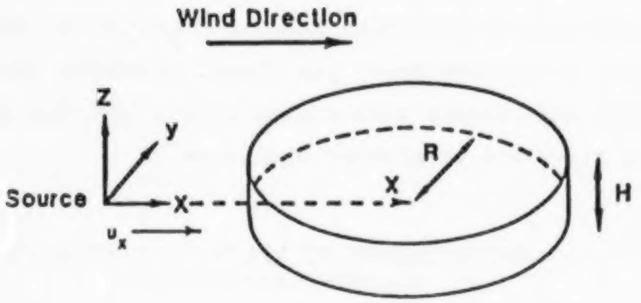


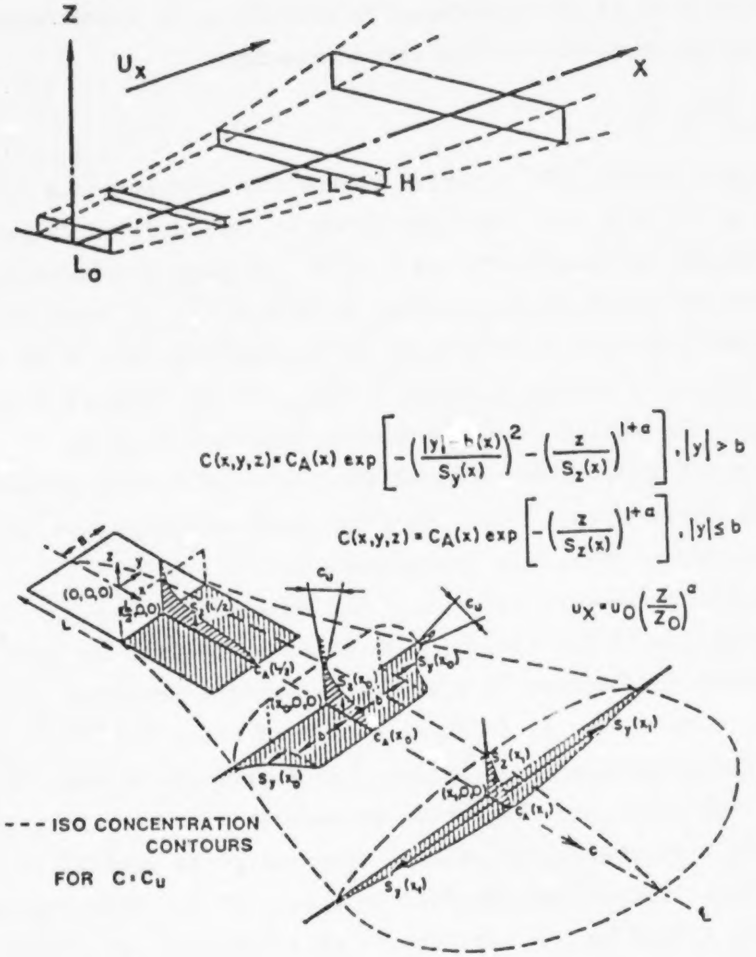
FIGURE 1. Cloud shape for instantaneous release.

represented as a vertically oriented cylinder, is placed in the flow field. The cloud is moved downwind with a velocity determined from the wind vertical profile. Figure 2 depicts the cloud shapes which have been most frequently used in models for continuous releases. The principal dimensions of the puff or plume change as a result of gravity spreading (assumed to occur crosswind only in the plume representation) and entrainment of air across the top and/or side boundaries.

Buoyancy-Dominated Flow Regime. For heavy gas releases with initially similar vertical and horizontal dimensions there is conclusive evidence that the rapid gravity-driven flow results in large-scale turbulent structures which effect rapid dilution of the cloud (11,12,13,14,15). Since this initial turbulent motion can result in a ten-fold to one hundred-fold dilution, it must be accounted for in heavy gas dispersion predictions. The lateral spreading that follows such releases is most frequently modeled as a gravity current with a frontal velocity calculated from the relation

$$u_f = C_E \, (g \, H)^{1/2} \tag{1}$$

Equation (1), which reflects the assumption of quasi-steady exchange of cloud potential and kinetic energy, indicates a



$$C(x,y,z) = C_A(x)\exp\left[-\left(\frac{|y| - h(x)}{S_y(x)}\right)^2 - \left(\frac{z}{S_z(x)}\right)^{1+a}\right], \ |y| > b$$

$$C(x,y,z) = C_A(x)\exp\left[-\left(\frac{z}{S_z(x)}\right)^{1+a}\right], \ |y| \le b$$

$$u_X = u_0\left(\frac{Z}{Z_0}\right)^a$$

FIGURE 2. Cloud shapes for continuous releases.

step change of the front velocity to its maximum value at the instant of release. The heavy gas must accelerate from rest, and van Ulden (16,17) and Meroney and Lohmeyer (18) have proposed methods for modeling the acceleration phase. Air entrainment at the spreading cloud front during the buoyancy-dominated flow is often modeled by specifying an entrainment velocity proportional to the front velocity:

$$u_e = C_1 u_f \qquad (2)$$

Havens and Spicer (19) reported laboratory instantaneous releases, in calm air, of right-circular cylinders of Freon-12 with initial volumes 0.035 and 0.51 m^3. Figure 3 summarizes the measured cloud front position (radius/$V^{1/3}$) vs. time (t/T). The cloud front position is well represented, for $t > \approx 20$ T, by the solution of Equation (1) with $C_E = 1.16$. Figure 3 also indicates the predicted cloud frontal position vs. time obtained using van Ulden's model for the acceleration phase. Figure 4 shows ground level, peak-measured concentration as a function of distance from the release center for the instantaneous Freon-12 releases. The volume-averaged concentrations of the clouds, determined by spatial integration of vertical and horizontal cloud concentration profiles, indicate a value for C_1 in Equation (2) of about 0.6.

Stably Stratified Flow Regime. An intermediate phase of the typical heavy gas dispersion process (between the buoyancy-dominated flow regime and passive dispersion) is similar to a stably stratified plume embedded in a mean flow. This regime is characterized by the persistence of a lateral (crosswind) gravity-driven flow and vertical density stratification which damps turbulent mixing. The lateral gravity spread can be modeled using Equation (1). The vertical mixing is usually modeled with a vertical entrainment velocity which is a function of the friction velocity of the flow and the

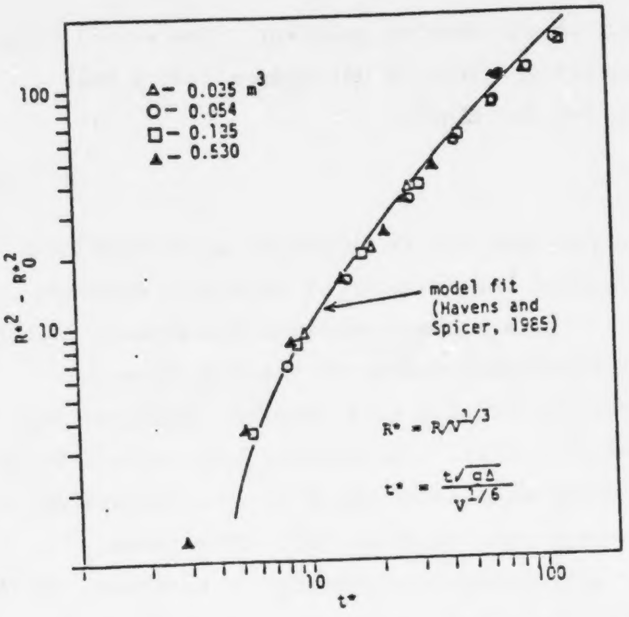


FIGURE 3. Cloud front position vs. time, Freon-12, H/D = 1.0, instantaneous release.

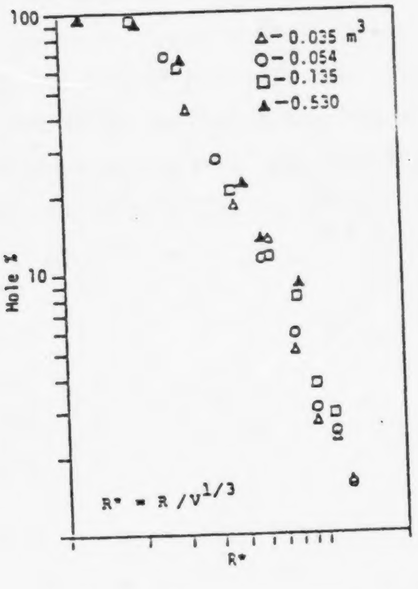


FIGURE 4. Maximum ground level concentration vs. distance. Freon-12, H/D = 1.0, instantaneous release.

stabilizing effect of the density gradient. The stabilizing effect of the density gradient is determined from a bulk Richardson number for the flow:

$$v_e = ku_*/\psi(Ri_*) \qquad (3)$$

The function ψ in Equation (3) is chosen to agree with laboratory experimental measurements of mixing in density-stratified flows. Figure 5 shows vertical entrainment velocity data vs. the bulk Richardson number of the flow from the experiments reported by McQuaid (20), Kantha, Phillips, and Azad (21), and Lofquist (22). The plotted line represents a curve fit of the three data sets, which cover a Richardson number range from near zero to about 10^5. This range encompasses heavy gas dispersion scenarios of interest. It is noted that questions have been repeatedly raised about the interpretation of both KPA's data and McQuaid's experiments, and there exist data reported by Ellison and Turner (23) and more recently by Deardorff (24), Kranenberg (25), and Stretch (26) which may justify some modification of the entrainment velocity specification shown in Figure 5. However, it is anticipated that such modifications would favor an increase in the entrainment velocity, and Figure 5 should reflect conservatism. Furthermore, modifications which may be necessary appear to be for higher Richardson numbers than are likely to be experienced in heavy gas dispersion scenarios of interest (27).

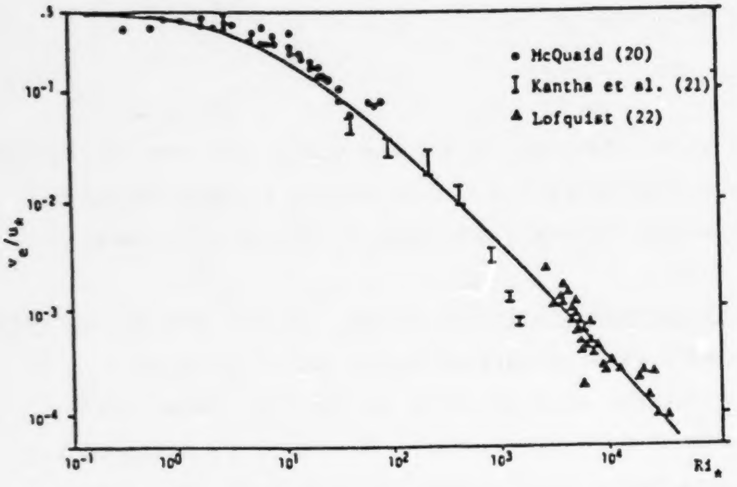


FIGURE 5. Correlation of vertical entrainment velocity with bulk Richardson number.

Passive Dispersion Regime. Vertical passive dispersion from ground level sources is conventionally modeled as a gradient transfer process by application of similarity principles developed by Monin (28) and Batchelor (29). The velocity profile in a stratified flow against a rough wall boundary is determined from

$$\frac{du_x}{dz} = \frac{u_*}{kz} \psi (z/\lambda) \qquad (4)$$

where the function ψ has been determined from experimental measurements of vertical momentum transfer by Businger (30). For the limiting case of neutral stratification, $\psi = 1$, and Equation (4) indicates a logarithmic velocity profile with roughness height z_r. The corresponding vertical diffusivity, defined as the ratio of momentum flux to the mean velocity gradient, is given by

$$K = \frac{k\, u_*\, z}{\psi} \qquad (5)$$

and (invoking the Reynolds analogy), the equivalent vertical entrainment velocity is

$$v_e = \frac{K}{z} \qquad (6)$$

For neutral stratification, $\psi = 1$ and $v_e/u_* = k$, the von Karman constant, which is about 0.4. This result is consistent with the extrapolation of data summarized in Figure 5 to zero Richardson number.

A General Purpose Similarity Model. Havens and Spicer (31) have developed a general purpose heavy gas dispersion similarity model for incorporation in the U.S. Coast Guard Hazard Assessment Computer System. The model is designed for simulating dispersion from ground level sources on water or level, unobstructed terrain. The DEGADIS (DEnse GAs DISpersion) model is an adaptation of the Shell HEGADAS model described by Colenbrander (32,33). The buoyancy-dominated flow regime is simulated using a box model to predict a "secondary" heavy gas source which is input to the downwind dispersion model. The box model of the buoyancy-dominated flow regime incorporates air entrainment at the gravity-spreading front based on the data correlation shown in Figures 3 and 4. The downwind dispersion phase of the calculation assumes a power law concentration distribution in the vertical and a modified Gaussian profile in the horizontal direction, with a power law specification for the wind profile. Vertical mixing (entrainment) is modeled using the data correlation shown in Figure 5. Horizontal dispersion in the stably stratified flow regime and the ensuing passive dispersion regime (a smooth transition, based on the vertical mixing data of Figure 5, is effected by the model) is forced to reflect experimental data on horizontal dispersion of passive plumes from point sources, such as the power law correlation of σ_y developed by Pasquill (34). DEGADIS provides for treatment of transient (including instantaneous) releases as a series of pseudo-steady state releases. The model also provides for heat transfer from the underlying surface to the cloud, as well as enhancement of vertical mixing by the unstable temperature gradient which results from heat transfer to the cloud. The convective turbulence is modeled using an approach adapted from Zeman and Tennekes (35).

DEGADIS has been used to simulate a wide range of field heavy gas releases, including small to intermediate LPG (0.1 to 1 kg/s) and LNG releases (1 to 100 kg/s) on land, large-scale releases (10 to 150 kg/s) of LPG and LNG on water, and instantaneous releases of approximately 5000 kg Freon/air mixtures on land. A comparison between the predicted and "observed" distance to the 5%, 2-1/2%, and 1% concentration levels for the Burro/Coyote, Maplin Sands, and Thorney Island field tests has been made. The observed values were determined from reported maximum concentrations for each experiment by drawing a visual best-fit straight line through the reported points in the concentration range of interest; all of the measurements used were made at heights at or below 1 m. The predicted distance to a given concentration level was based on the ground level centerline concentration calculated by DEGADIS; for the concentrations and conditions of interest, the predicted concentration level is essentially constant for heights below 1 m. From these values, a ratio of the observed to the predicted distance for each experiment was calculated. Table I summarizes ratios of the observed to predicted distances for the concentration levels of interest. As well, a 90% confidence interval of these ratios is included for each test series and for all of the experiments together. (For instance, the Maplin Sands comparisons indicate the ratio of the observed to the predicted distance to the 2-1/2% concentration level would be between 0.91 and 1.20 in nine out of ten realizations.) For all of the comparisons in Table I, the ratio of observed distance (OBS) to predicted distance (PRE) for a given ensemble-averaged concentration level ranged from 0.73 to 0.96 for the 5% level nine out of ten times (i.e.

TABLE I. Comparison between "Observed" and DEGADIS-Predicted Maximum Distance to Gas Concentrations in the Flammable Concentration Range.

	Ratio of "Observed" Distance to DEGADIS-Predicted Distance $(OBS/PRE)_y$ for the Concentration Level y:		
Test Series	y = 5%	y = 2.5%	y = 1%
Thorney Island 7	1.17	1.12	0.63
8	1.09	0.90	0.66
9	1.00	0.95	1.28
11	0.55	0.61	0.63
13	0.70	0.70	0.70
15	1.05	0.90	0.77
Thorney Island 90% Confidence Interval	$0.71 \le (OBS/PRE)_5 \le 1.11$	$0.70 \le (OBS/PRE)_{2.5} \le 1.02$	$0.64 \le (OBS/PRE)_1 \le 0.99$
Maplin 22	0.47	0.64	1.15
27	0.95	1.10	1.46
29	0.89	0.96	1.20
34	1.28	1.38	1.76
35	1.28	1.59	2.61
39	0.46	0.63	1.21
43	0.73	0.84	0.91
46	1.09	1.17	1.33
47	0.77	0.92	1.06
49	1.27	1.35	1.46
50	0.92	0.90	1.26
54	1.12	1.21	1.19
56	0.93	0.92	1.02
Maplin 90% Confidence Interval	$0.80 \le (OBS/PRE)_5 \le 1.10$	$0.91 \le (OBS/PRE)_{2.5} \le 1.20$	$1.15 \le (OBS/PRE)_1 \le 1.47$
Burro 3	0.52	0.69	0.83
7	0.63	0.74	0.95
8	0.93	1.21	1.66
9	0.51	0.78	1.22
Coyote 5	0.75	0.71	0.71
6	0.38	0.38	0.43
Burro 90% Confidence Interval	$0.46 \le (OBS/PRE)_5 \le 0.78$	$0.55 \le (OBS/PRE)_{2.5} \le 0.98$	$0.63 \le (OBS/PRE)_1 \le 1.31$
Summary 90% Confidence Interval	$0.73 \le (OBS/PRE)_5 \le 0.96$	$0.82 \le (OBS/PRE)_{2.5} \le 1.03$	$0.95 \le (OBS/PRE)_1 \le 1.24$
Summary 99% Confidence Interval	$0.64 \le (OBS/PRE)_5 \le 1.03$	$0.78 \le (OBS/PRE)_{2.5} \le 1.09$	$0.88 \le (OBS/PRE)_1 \le 1.33$

90% confidence interval); for the 2.5% level, (OBS/PRE) ranged from 0.82 to 1.03 for a 90% confidence interval; for the 1% level, (OBS/PRE) ranged from 0.95 to 1.24 for a 90% confidence interval.

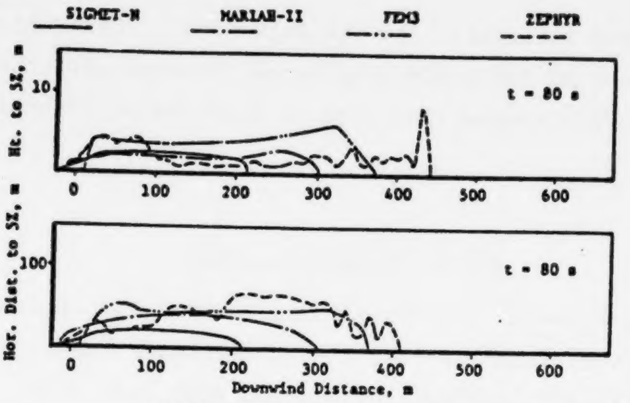
3-D Mathematical Models

The Gas Research Institute in the United States is sponsoring a research project (36) to evaluate the SIGMET-N (37), ZEPHYR (38), MARIAH-II (39), and FEM3 (40) 3-D mathematical models for LNG vapor dispersion. 3-D mathematical models have been also reported by Schreurs (41), Rioux (42), Betts et al. (43), and Deaves (44). These models have had limited use, partly because of hesitation by regulatory authorities to allow their use without a thorough technical evaluation.

Comparison simulations were made in the GRI evaluation project with SIGMET-N, ZEPHYR, MARIAH-II, and FEM3 of the Burro 9 LNG spill test (7). Figure 6 shows the centerline vertical and one meter elevation horizontal 5% gas concentration contours predicted at 80 seconds from spill start by the four models. (Also shown are the grid cell sizes used, the total number of cells computed, and the VAX 11-730 cpu time required for the models.) Important differences were observed in the predicted maximum downwind extent as well as the maximum lateral extent of the LFL contour. These differences were attributed primarily to two factors:

- numerical diffusion (truncation) errors
- turbulent mixing (closure) models

The model evaluation program has focused on these two model characteristics.



	LFL Dist, m	Δx, m	Δy, m	Δz, m	Cells	cpu, h
ZEPHYR	>440	10	.67	6	11,250	173
SIGMET-N	215	10	.67	6	11,250	79
MARIAH-II	310	10	.67	6	11,250	6.4
FEM3	375	*	*	*	3,680	~60

*variable, expanding grid

FIGURE 6. Comparison predictions of vertical centerline and one meter height horizontal 5% gas contours--Simulation of Burro 9 experiment with four models.

Numerical Diffusion Properties. The numerical solution of advection-diffusion equations (the momentum, mass, and energy balance equations) using finite differences or elements results in truncation errors which cause a "numerical diffusion" component in the solution (45). The numerical diffusion errors must be maintained small compared to the contributions from the actual diffusion terms in the balance equations. The severity of numerical diffusion depends on the finite difference scheme used and the discretization (spatial step size).

The SIGMET-N model uses first-order, forward-time, centered space finite differences for the advection terms of all balance equations. The method used is equivalent to using "upwind" differencing, and test calculations for representative heavy gas dispersion scenarios demonstrate the severity of numerical diffusion (Havens and Schreurs, 46).

ZEPHYR uses second-order, centered-space finite differences for the advection terms in the momentum balance equations. The contaminant gas balance equation is simulated with a Lagrangian model in which particles representing the contaminant gas are transported in the finite difference grid by advection at the local (interpolated) flow velocity and diffused via a random walk prescription. The particle treatment of the gas contaminant balance equation effectively avoids the problem of numerical diffusion. However, the random walk method used to simulate the turbulent mixing (diffusion) of the gas is not suitable for application to the strongly varying diffusivity field which is expected in an LNG vapor cloud (Schreurs et al. (47)).

MARIAH-II uses a second-order Crowley difference approximation for the advection term in the gas contaminant balance equation. This method substantially reduces numerical diffusion errors but can result in oscillatory behavior in regions of high concentration gradients. In MARIAH-II these oscillations are identified and locally damped using Chapman's FRAM (filtering remedy and methodology) method (48).

FEM3 uses finite elements to approximate the spatial variation of the problem variables. With the first-order function approximations which have been used in applications to LNG vapor dispersion, FEM3 can be compared to the finite difference methods.

An extensive computational exercise to evaluate the numerical diffusion properties of the four models being evaluated in the GRI project has been reported by Havens and Schreurs (49). Based on the results, it was determined that satisfactory control of numerical diffusion errors in LNG vapor dispersion predictions was not practical with the SIGMET-N model, and it has not been evaluated further. The numerical diffusion properties of the ZEPHYR model and the development efforts which would be required to adapt (and verify) the Langrangian particle treatment of turbulent gas mixing for the typical heavy gas dispersion scenario also led to its elimination from the evaluation project. The evaluation of MARIAH-II and FEM3 has continued, with emphasis on testing by comparison with wind tunnel test data which reflect strong density stratification effects and for which the turbulent mixing can be quantified. Particular use has been made of two wind tunnel heavy gas release data sets:

- two-dimensional, continuous, heavy gas releases in a wind tunnel
- three-dimensional, continuous, heavy gas releases in a wind tunnel. In the experiments selected for analysis, the dispersion appears to have been confined to a zone adjacent to the wind tunnel floor where turbulence was damped and the mixing was essentially molecular (50,51).

McQuaid (20) reported measurements of the vertical dispersion of carbon dioxide ($\rho/\rho_a = 1.52$) introduced as a floor level, near-line source in a fully developed wind tunnel flow of width 0.3 m, height 0.9 m, and working length 5.5 m. The mean velocity, u_a, in the tunnel ($\approx 0.8\ u_{max}$) ranged from 0.82 to 3.52 m/s. The friction velocity (in the absence of any dense gas) was reported as $u_* = 0.0412\ u_a$. The Reynolds number (based on the mean velocity and the tunnel hydraulic diameter) ranged correspondingly from 2.5×10^4 to 1.1×10^5. Three of McQuaid's experiments have been selected for simulation. The conditions for the three experiments, which were chosen to represent near-passive dispersion to stably stratified flow dispersion, are given in Table II.

TABLE II. Summary of Experimental Conditions--McQuaid (20)

	Experiment		
	1	2	3
Average velocity over channel (m/s)	3.6	1.83	1.28
Friction velocity (m/s)	0.144	0.073	0.05
Source strength (kg/m s)	0.0113	0.0142	0.0226
Source exit (vertical) velocity (m/s)	0.124	0.155	0.248
Richardson number[1] range	0.5-0.9	4.0-8.0	28.0-44.0
Gas density (kg/m^3)	1.83	1.83	1.83
Source dimensions width, m - length, m	0.3-0.05	0.3-0.05	0.3-0.05
Roughness length (m) (calculated from velocity profile)	1×10^{-5}	1×10^{-5}	1×10^{-5}

[1] $Ri_* = g \frac{\Delta\rho}{\rho_a} \frac{H_{eff}}{u_*^2}$

McQuaid's experiments have been used to evaluate numerical diffusion in the MARIAH-II and FEM3 models in an indirect way. McQuaid has shown that the vertical gas concentration distributions in the three experiments chosen for evaluation are well represented as Gaussian. The measured gas concentration distribution has been used to estimate the vertical air entrainment velocity and a diffusivity profile consistent with the measurements specified. This approximate knowledge of the "correct" turbulent eddy diffusivity for these experiments allows comparison calculations with either zero (MARIAH-II) or very small (FEM3) diffusivities to determine the relative importance of numerical vs. "physical" diffusion. These computations have also been reported (49). For the three experiments chosen for analysis, which represent near-passive to strongly stratified flow dispersion, the slope of the maximum (ground level) concentration vs. distance which is attributable to numerical diffusion is satisfactorily small compared to the experimentally observed concentration decay.

Kothari and Meroney (KM) (50) and Meroney and Neff (MN) (51) reported measurements of the lateral gravity spread and dispersion of isothermal heavy gases released continuously from floor level area sources in an unobstructed wind tunnel flow. Two experiments have been carefully studied. Table III lists the experimental conditions of KM 75 and MN 42. It appears that in these two experiments the heavy gas dispersion processes were confined to the zone adjacent to the wind tunnel floor where mixing was molecular. Accordingly, both experiments were simulated using the molecular diffusivities for the gases involved (CO_2 and Argon, respectively) for the diffusion calculation.

Figure 7 compares the measured and predicted ground level centerline gas concentration and the ground level horizontal concentration distributions at four downwind distances for KM 75 using MARIAH-II and for MN 42 using MARIAH-II and FEM3. Since these three-dimensional experiments involve gas flows

TABLE III. Summary of Experimental Conditions--
Kothari-Meroney (50) and Meroney-Neff (51)

	KM 75	KM 42
Tunnel velocity (m/s)	0.24 @ 0.4 m	0.20 @ 2.1 cm
Friction velocity (m/s)	0.017	0.015
Source strength (kg/s)	2.68×10^{-4}	2.77×10^{-4}
Source exit velocity (m/s)	2.11×10^{-3}	9.6×10^{-3}
Gas density (kg/m^3)	1.82 (CO_2)	1.63 (Argon)
Source diameter (m)	0.3	0.15
Roughness length (m)	0.00015	0.0001
Gas molecular diffusivity (m^2/s)	1.5×10^{-5}	1.5×10^{-5}

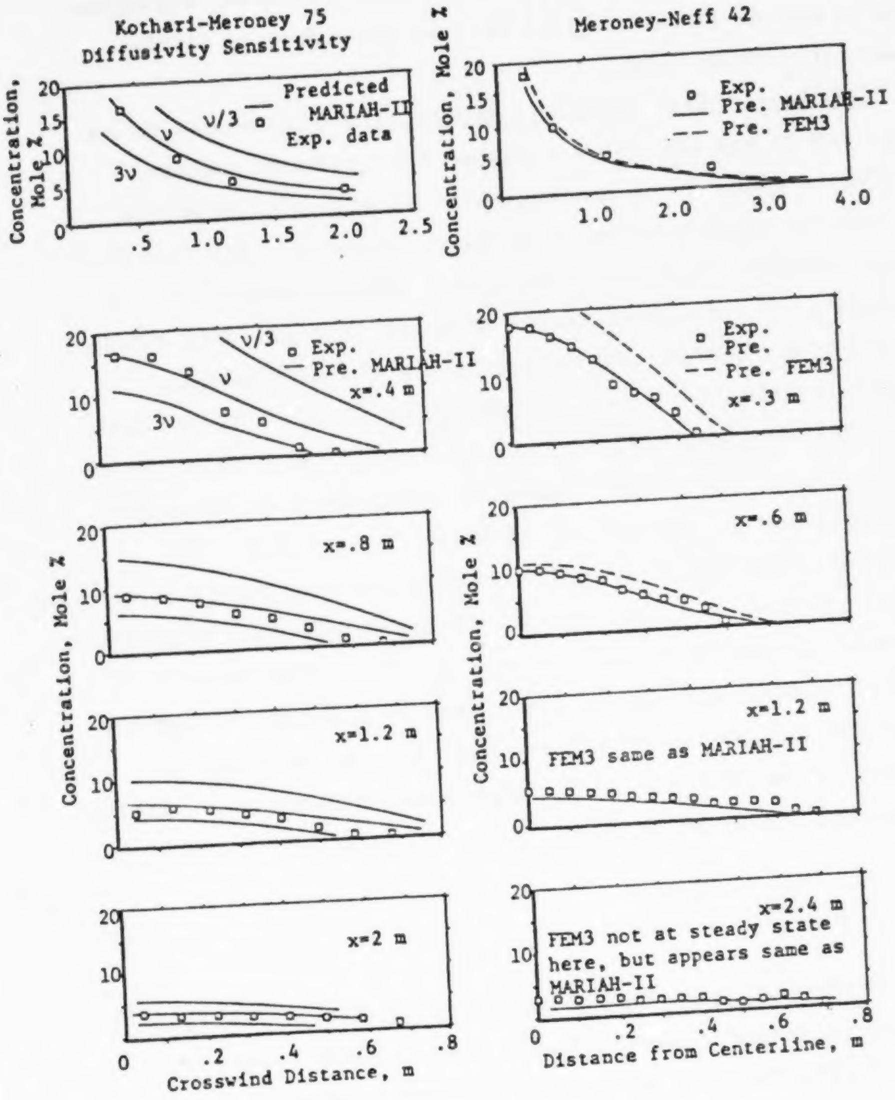


FIGURE 7. Comparison of measured and predicted gas concentrations for Kothari-Meroney 75 and Meroney-Neff 42.

with a strong lateral gravity-driven component, and since the molecular diffusion coefficient is well known, the agreement of these simulations with the experimental data provides important assurance of the general applicability of the model equations used in MARIAH-II and FEM3 as well as the adequacy of the numerical methods used.

Turbulent Mixing (Closure) Models. The four models being evaluated in the GRI project assume the gradient transfer hypothesis with ad hoc specification of eddy diffusivities. The primary specification is of eddy diffusivity for transfer in the vertical direction; horizontal diffusivities are obtained from prescribed ratios with the vertical diffusivity.

SIGMET-N, ZEPHYR, and MARIAH-II use the diffusivity specification method incorporated in the original SIGMET model (52). The vertical diffusivity is specified as a function of height, "local stability" (based on temperature or density gradient), and local velocity as shown in Figure 8. The selection of a "local" Pasquill stability category is based on the correlation of stability with vertical temperature gradient specified in the USAEC Safety Guide 23 (53). The Pasquill stability categories can be correlated with a bulk Richardson number for the atmospheric flow (54), and the vertical diffusivity coefficient can be expressed in terms of a vertical entrainment velocity, v_e', as

$$K_y = \frac{k\, u_* \, y}{\phi(Ri_*)} = \frac{v_e' \, y}{1 + \alpha} \qquad (7)$$

Figure 9 shows representative values of nondimensionalized vertical entrainment velocity with these models, based on Equation (7), for bulk Richardson numbers greater than 0.1. Figure 9 also shows nondimensionalized vertical entrainment velocity as a function of bulk Richardson number (data points) obtained from analysis of the laboratory stratified fluid mixing experiments of McQuaid (20); Kantha, Phillips, and Azad (21); and Lofquist (22). The solid line curve plotted on

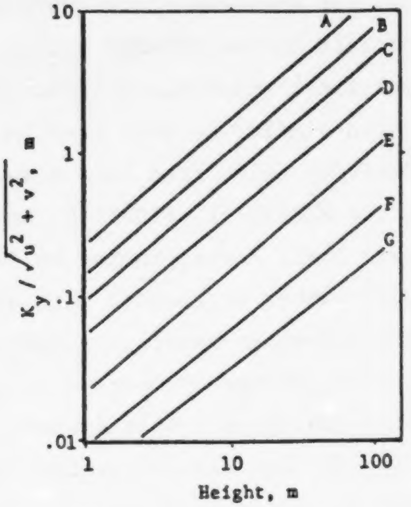


FIGURE 8. Vertical diffusivity specification in MARIAH-II, SIGMET-N, and ZEPHYR.

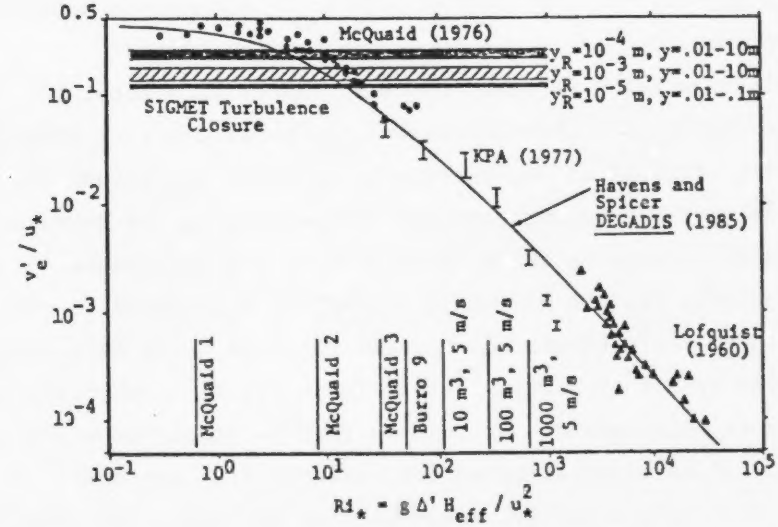


FIGURE 9. Vertical entrainment as a function of bulk Richardson number.

Figure 9 is a curve fit (of the laboratory experimental data) which has been incorporated in the DEGADIS model. The DEGADIS correlation of nondimensional entrainment velocity with bulk Richardson number is also similar to that used in FEM3.

The vertical diffusivity calculated in a simulation of LNG vapor dispersion with the MARIAH-II, SIGMET-N, and ZEPHYR models will have a lower limit corresponding to "G" stability when the bulk Richardson number is greater than about 0.1, and there is no provision for further damping of turbulence which would be indicated for the stronger temperature (and density) gradients expected in an LNG cloud. Bulk Richardson numbers, based on release conditions, can also be estimated to characterize laboratory and field experiments. Figure 9 indicates the Richardson numbers estimated for three wind tunnel heavy gas releases reported by McQuaid (20), the Burro 9 field experiment, and continuous LNG releases of 160, 980, and 5250 kg/s (representing maximum source rates from instantaneous LNG spills onto water of 10, 100, and 1000 m^3 respectively) in a 5 m/s wind. There is a clear indication that the turbulent mixing model used in MARIAH-II, SIGMET-N, and ZEPHYR will tend to give too low vertical diffusivities for Richardson numbers between about 0.1 and about 20, and too high vertical diffusivities for Richardson numbers greater than about 20. It is also significant that the turbulence model may fortuitously represent vertical mixing reasonably well for Ri_B around 30, which is probably appropriate for characterizing the Burro 9 experiment. Based on these observations, the turbulence closure model used in MARIAH-II, SIGMET-N, and ZEPHYR is not expected to scale adequately for LNG releases which have widely different ratios of vertical shear (high friction velocity) and density stratification. It follows that vertical turbulent mixing will be underestimated for releases with low bulk Richardson numbers and overestimated for releases with large bulk Richardson numbers. The former cases include many small-scale wind tunnel experiments, and the latter include large LNG releases in low-wind conditions, such as Burro 8. The underestimation of vertical diffusivities for the small-scale McQuaid 2-D wind tunnel heavy gas experiments has been demonstrated by Havens and Schreurs (46).

A simplified second-order turbulence model has been developed by Freeman (47) for simulation of LNG vapor cloud dispersion. The principal simplifying assumptions invoked in the model are:

- The theory is local; all turbulent quantities are assumed point functions depending only on the state of the mean field.
- The mean field employed in the turbulence terms is simplified to retain the dominant terms describing a stratified boundary layer; turbulent kinetic energy is dependent on the magnitude of the shear of the flow field

$$S = [(\partial u/\partial y)^2 + (\partial w/\partial y)^2]^{1/2}$$

and the gradient Richardson number

$$Ri = - \frac{g(\partial \rho/\partial y)}{\rho S^2}$$

MARIAH-II with the turbulence closure method developed by Freeman and modified to provide for turbulence kinetic energy diffusion has been used to simulate McQuaid's experiments. Figure 10 shows the experimental vs. MARIAH-II-predicted ground level gas concentration decay with distance. The agreement is now reasonably good for all three experiments.

MARIAH-II, with Freeman's turbulence closure model, has also been used to simulate Havens' and Spicer's laboratory instantaneous releases of heavy gas. Figure 11 shows a MARIAH-II simulation of a 55-liter Freon release with an initial height-to-diameter ratio of 1.0. The cloud profile (half of the radially symmetric section of the cloud is shown), defined by the 1% volume fraction, is shown at zero time and at 0.5, 1, 2, 3, 4, 5, and 6 seconds after release. Figure 12 shows the

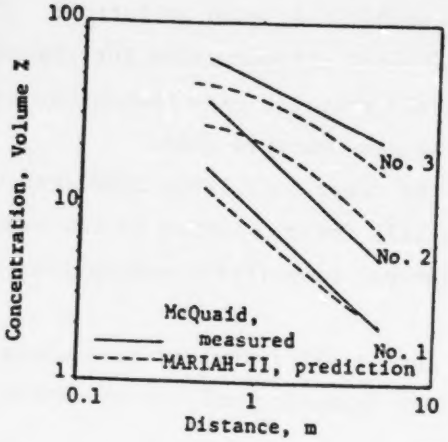


FIGURE 10. McQuaid 2-D wind tunnel experiments--MARIAH-II predictions with improved air entrainment model.

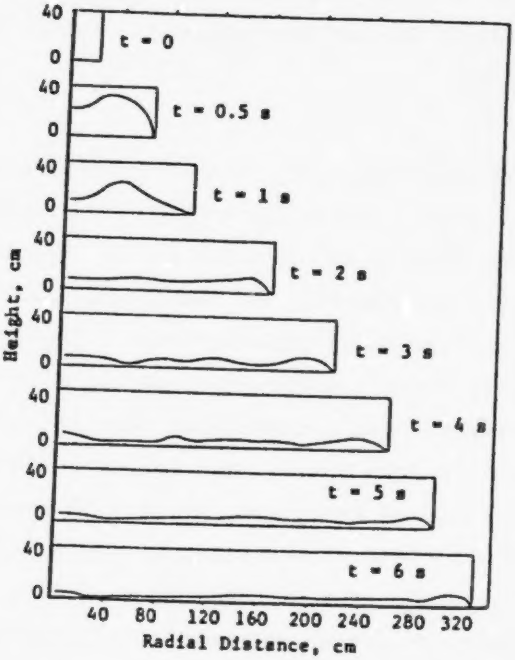


FIGURE 11. Laboratory, calm-air, 55-liter Freon release, $(H/D)_i$ = 1.0--MARIAH-II prediction of cloud boundary vs. time.

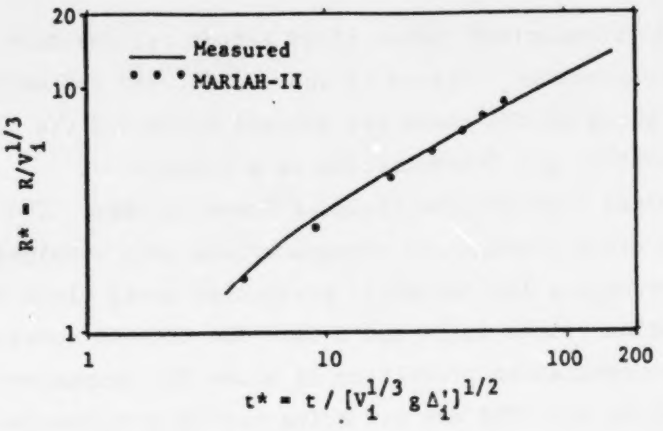


FIGURE 12. Laboratory, calm-air, 55-liter Freon release, (H/D)$_i$ = 1.0--MARIAH-II prediction of cloud radial extent.

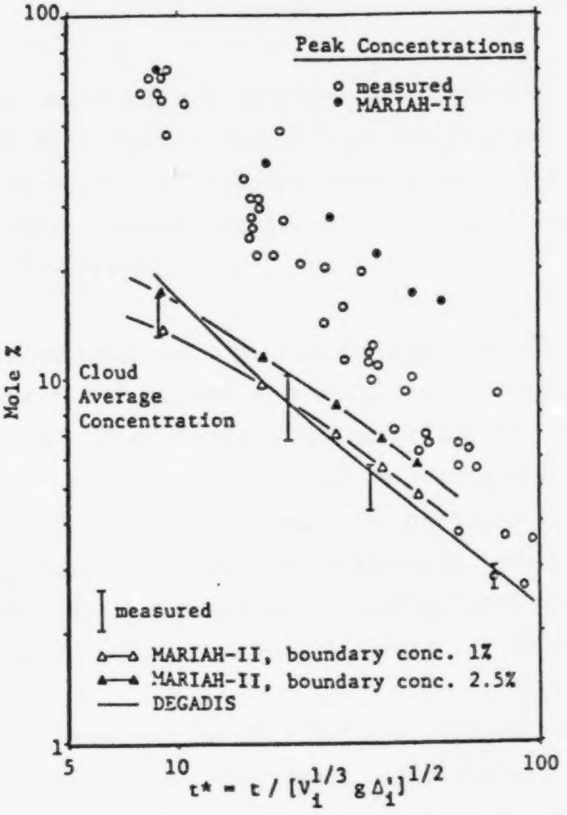


FIGURE 13. Laboratory, calm-air, 55-liter Freon release, (H/D)$_i$ = 1.0--Measured and predicted cloud maximum and volume-averaged gas concentrations.

predicted vs. measured radial cloud extent for the same 55-liter Freon release. Figure 13 shows predicted and measured maximum values of the cloud gas concentration and the cloud spatial average gas concentration as a function of dimensionless time for the 55-liter Freon release. The predicted cloud average gas concentrations were obtained by spatial averaging the MARIAH-II prediction using cloud boundary concentration limits of 1% and 2.5%. The DEGADIS model cloud average concentration prediction is shown for comparison (31).

MARIAH-II and FEM3 are now being tested by comparison with selected data from the Burro/Coyote, Maplin Sands, and Thorney Island experiments.

CLOSURE

Similarity models are available for heavy gas releases at ground level on uniform terrain with unobstructed atmospheric flow. Some models have been verified for the prediction of dispersion to flammable concentration levels (order 1%) and are sufficiently accurate for most risk assessment and emergency response applications.

Most field heavy gas dispersion tests have provided data on cloud dispersion to fuel flammable-limit concentration levels; such data are not sufficient to verify models for application to toxic gas dispersion to parts per million concentration levels. It is expected that models which have been verified for flammable fuel dispersion prediction and also incorporate an appropriate description of the passive dispersion regime should be useful for prediction of dispersion of dense gases to toxicity levels.

It appears likely that 3-D mathematical models can be verified for flammable gas dispersion prediction, but current work is biased strongly toward evaluation using data without terrain or wake turbulence effects. Since the primary motivation for using these models is to describe such complex effects, research should be directed to their validation for such use.

3-D mathematical models are not likely to prove useful for predicting heavy gas dispersion to very low concentration levels because of difficulties in managing numerical diffusion in calculations with several orders of magnitude change in concentration.

Application of dense gas dispersion models to toxic gas dispersion is expected to require additional research to provide for description of jetting releases, aerosol formation and evaporation, chemical reaction, and deposition.

The participants in the recent joint EPA-DOE workshop agreed that source specification in an accident may be a greater concern than the accuracy of a dispersion model. A technology transfer problem was identified; many of the improvements in dispersion models have not been transferred to the potential user. There was a consensus that atmospheric dispersion predictions should be done to plan emergency response whenever possible. No selection or recommendation of models was made.

LIST OF SYMBOLS

C_E	constant in density intrusion (spreading) relation
C_1	constant
g	acceleration of gravity (m/s^2)
H	height or depth of density intrusion or cloud (m)
H_{EFF}	effective cloud depth (m)
K	vertical turbulent diffusivity (m^2/s)
k	von Karman's constant, 0.35

Ri_*	Richardson number associated with density differences
T	characteristic time scale, $V^{1/6}/\sqrt{g(\rho - \rho_a)/\rho_a}$
t_f	characteristics time of cloud formation (s)
t_t	cloud travel time to the maximum distance exposed to a given concentration (s)
u	velocity along x-direction, (m/s)
u_a	ambient average velocity, (m/s)
u_e	horizontal or frontal entrainment velocity, (m/s)
u_f	cloud front velocity, (m/s)
u_x	wind velocity, along x-direction, (m/s)
u_{max}	maximum velocity
u_*	friction velocity, (m/s)
V	cloud volume, (m^3)
v_e	vertical entrainment velocity associated with H_L, (m/s)
w	velocity along z-direction, (m/s)
x,y,z	Cartesian coordinates, (m)
α	constant in power law wind profile
λ	Monin-Obukhov length (m)
ρ	density (kg/m^3)
ρ_a	ambient density (kg/m^3)
σ_y	Pasquill-Gifford lateral dispersion coefficient (m)
ϕ	function describing influence of stable density stratification on vertical diffusion
ψ	logarithmic velocity profile correction function

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APPENDIX D

Workshop Agenda

AGENDA

Determination of Atmospheric Dilution for Emergency Preparedness
A Joint EPA-DOE Technical Workshop
October 15-17, 1986

TIME	TOPIC	SPEAKER
Wednesday, October 15, 1986	Meredith Guest House Research Triangle Park, NC	
SESSION 1		
8:00 - 8:10 a. m.	Welcome	Frank Binkowski, USEPA & NOAA and Harry Moses, USDOE
8:10 - 8:40 a. m.	Technical Overview	R. A. Cox, Technica
Two Recent Catastrophic Events		
8:40 - 9:00 a. m.	Bhopal	Shankar Rao, NOAA/ATDD
9:00 - 9:20 a. m.	National Research Needs for Emergency Response in the Wake of Chernobyl	Joe Knox, Lawrence Livermore Laboratory
SESSION 2 Characteristics of Sources of Releases of Toxic Material Chairman: Joe Knox, Lawrence Livermore Laboratory		
9:20 - 9:40 a. m.	Historical Accounts and Credible Scenarios	Jane Crum, Bob Hangebrauck, and Bill Rhodes, USEPA
9:40 - 10:00 a. m.	Short Term Toxic Releases from Industrial Sites	Robert Rosensteel, USEPA
10:00 - 10:20 a. m.	Fate of Toxic Releases in the Atmosphere - ARAC	Marvin Dickerson, LLL
10:20 - 10:40 a. m.	Source Strength Modeling	Jerry Schroy, Monsanto
SESSION 3 Regulatory and Operational Needs for Models Chairman: Bob Hangebrauck, USEPA		
10:40 - 11:00 a. m.	Future Needs for Dispersion Models in Hazard Evaluation,	Jim Makris, USEPA

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TIME	TOPIC	SPEAKER
SESSION 3 (Cont'd)		
	Emergency Preparedness, and Accident Prevention	
11:00 - 11:20 a. m.	Issues in Regulatory Applications of Models	Dave Layland, USEPA
11:20 - 11:40 a. m.	Community Needs for Hazard Evaluation Tools	Fred Millar, Environmental Policy Institute
11:40 - 1:00 p. m.	Lunch	
SESSION 4 Dispersion Models Chairman: Dick Benjamin, Savannah River Laboratory		
1:00 - 1:30 p. m.	Keynote Talk	Jerry Havens, University of Arkansas
1:30 - 1:50 p. m.	Dense Gas Dispersion Model	Don Ermak, LLL
1:50 - 2:10 p. m.	Reactive Dense Gas Models	Bruce Hicks and Will Pendergrass, NOAA/ATTD
2:10 - 2:30 p. m.	Dispersion Models for Neutrally Buoyant and Positively Buoyant Gases	Tom Pierce, USEPA & NOAA
2:30 - 2:45 p. m.	Break	
SESSION 5 Results from Dispersion Experiments Chairman: Ray Hosker, NOAA/Atmospheric Turbulence & Diffusion Division		
2:45 - 3:05 p. m.	Laboratory Scale Experiments	Bob Meroney, Colorado State University
3:05 - 3:25 p. m.	Experimental Work at the EPA Fluid Modeling Facility	Bill Snyder, USEPA & NOAA
3:25 - 3:45 p. m.	Large Scale Experiments of the DOE Liquefied Gaseous Fuels Program	Ron Koopman, LLL

TIME	TOPIC	SPEAKER
3:45 - 4:05 p. m.	Atmospheric Science and Emergency Response at the Savannah River Plant	Alan Weber, Savannah River Laboratory
4:05 - 4:42 p. m.	Emergency Preparedness and Response in the U. S. Air Force	Larry Key, USAF
Thursday, October 16, 1986		
SESSION 6 Panel Discussions		
8:00 - 11:30 a. m. (Break 9:30 - 9:45 a. m.)	Summary of Current Status of Source Strength and Dispersion Models, Their Strengths and Weaknesses, and Recommendations for Improvement	Panel 1 Chairman: Frank Schiermeier Reporter: Steve Perry
1:00 - 3:30 p. m.	Recommendations for Selection from Among Current Models for Immediate Use in Hazard Identification and Evaluation, Preparation of Emergency Preparedness Scenarios, and in Response to Emergencies	Panel 2 Chairman: Ray Hosker Reporter: Tom Pierce
3:30 - 3:45 p. m.	Break	
3:45 - 5:00 p. m.	The Role of the Meteorologist in Hazard Evaluation, Emergency Response	Chairman: Lew Nagler Reporter: Jack Shannon
Friday, October 17, 1986		
8:00 - 11:30 a. m. (Break 9:30 - 9:45 a. m.)	Presentation of Results of Panel Discussions	

APPENDIX E

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DETERMINATION OF ATMOSPHERIC DILUTION FOR EMERGENCY PREPAREDNESS
A JOINT EPA-DOE TECHNICAL WORKSHOP
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